Blanch remlte

L4 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:348803 CAPLUS Full-text

DN 138:354008

TÍ Synthesis of diazabicycloalkanecarboxamides as caspase inhibitors

IN Robidoux, Andrea L. C.; Wilson, Jeffrey Douglas; Dieterich, Petra; Storer, Neil; Leonardi, Stefania

PA Vertex Pharmaceuticals Incorporated, USA

SO U.S., 14 pp., Cont.-in-part of U.S. 6,201,118. CODEN: USXXAM

DT Patent

LA English

FAN CNT 3

PATENT NO.		KIND	DATE		APPLICATION NO.		DATE
							
PI US	6559304	В1	200305	506	US	2000-688301	20001013
US	6201118	B1	200103	313	US	1998-136339	19980819
PRAI US	1998-136339	A2	199808	319			
OS CAS	SREACT 138:354	008; M	IARPAT 1	L38:354008			
GI							

- Diazabicycloalkanecarboxamides I [m = 0-2; n = 0, 1; X = CH, N; R = H, aryl, acyl, (un)substituted alkyl, CO2H, SO2H, CONH2, SO2NH2; R1 = OH, CF3, COCO2H, CO2H, (un)substituted alkyl; R2 = CN, (un)substituted CH:CH2, CH:NOH, alkyl, acyl, COCONH2] were prepared as known caspase inhibitors. Thus, the pyridazodiazepinecarboxamide II was prepared from Br(CH2)4CO2H in 9 steps.
- IT 192756-07-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of diazabicycloalkanecarboxamides as caspase inhibitors)

RN 192756-07-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1-isoquinolinylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,(3S)- (9CI) (CA INDEX NAME)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
     ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     2001:816645 CAPLUS Full-text
     135:344728
DN
     Asymmetric synthesis of piperazic acid and derivatives
ΤI
     Robidoux, Andrea; Serafini, Siro; Dieterich, Petra; Leonardi, Stephania;
IN
     Stibbard, John
     Vertex Pharmaceuticals Incorporated, USA
PA
     PCT Int. Appl., 51 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 1
                      KIND
                            DATE
                                            APPLICATION NO.
     PATENT NO.
                       A2
                            20011108
                                            WO 2001-US13330
                                                             20010425
PΙ
     WO 2001083458
                       Α3
                            20020523
     WO 2001083458
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                       A2
                           20030205
                                           EP 2001-930747
                                                            20010425
     EP 1280780
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                            20030918
                                            US 2002-168463
                                                             20020614
     US 2003176691
                       A1
                       B2
                            20031014
     US 6632942
PRAI US 2000-202104P
                       Ρ
                            20000504
                       W
                            20010425
     WO 2001-US13330
     CASREACT 135:344728; MARPAT 135:344728
os
GΙ
 R^1
      Piperazic acids I [R is H or a carboxy-protecting group; R1, R2 = H or
AΒ
      anamino protecting group; R1 and R2 may be taken together to form a
      fused bicyclic or tricyclicamino protecting group (R1 = R2 ≠ H)] were
      prepared by treating R40(CH2)3CH(OR4)CO2R (OR4 is a leaving group) with
      hydrazines R1NHNHR2 in the presence of a base and an organic solvent.
      Thus, treating a solution of CbzNHNHCbz (Cbz = PhCH2O2C) and (R)-tert-Bu
      2,5-dimesylvalerate in DMF with Na2SO4 and TBAF and stirring the mixture
      at room temperature for 24 h afforded (S)-tert-Bu 1,2-
     bis (benzyloxycarbonyl) hexahyd ro-3-pyridazinecarboxylate.
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (asym. synthesis of piperazic acid and derivs.)
RN
     192756-07-3 CAPLUS
CN
     Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1-
     isoquinolinylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-
     a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,(3S)- (9CI) (CA INDEX NAME)
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Absolute stereochemistry.

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ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     2001:489403 CAPLUS Full-text
DN
     135:92659
     Preparation of carboxamide diazepin derivatives and their inhibition of
ΤI
     cathepsin K, cathepsin B, and papain
     Bhatnagar, Neerja; Mauger, Jacques
IN
    Aventis Pharma S.A., Fr.
PA
SO
     PCT Int. Appl., 231 pp.
    CODEN: PIXXD2
DT
     Patent
LA
     French
FAN.CNT 1
                            DATE
                                            APPLICATION NO.
     PATENT NO.
                      KIND
    WO 2001047930
                       A1
                            20010705
                                           WO 2000-FR3622
                                                             20001221
PΤ
            AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CR, CU, CZ, DM, DZ,
             EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT,
             LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TT, UA, US,
             UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     FR 2802927
                       A1
                            20010629
                                           FR 1999-16567
                                                             19991228
     FR 2802927
                       В1
                            20020301
                                            EP 2000-990087
                                                             20001221
     EP 1246824
                       A1
                            20021009
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
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                            20021015
                                            BR 2000-16845
     BR 2000016845
                      , A
                                            JP 2001-549400
                                                             20001221
     JP 2003519152
                       Т2
                            20030617
                       Α
                            20030815
                                            EE 2002-362
                                                             20001221
     EE 200200362
                                            NO 2002-3107
                                                             20020627
                       Α
                            20020827
     NO 2002003107
                                            US 2002-168116
                                                             20020708
                       A1
                            20030529
     US 2003100550
                       Α
                            19991228
PRAI FR 1999-16567
                       W
                            20001221
     WO 2000-FR3622
     MARPAT 135:92659
OS
GΙ
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$$\begin{array}{c|c}
 & \circ \\
 & \downarrow \\$$

The title compds. I [R1 = C(0), R5, SO2R5, C(0)NR6R5; R2 and R7 are such that either R7 represents a hydrogen atom and R2 is such that the group (a) represents the radical of a natural or nonnatural amino acid, or R2 and R7 form together a cycle with the nitrogen and carbon atom whereto they are bound; R3 = CH:N2 or CH2LR4, R4 represents in particular a linear or branched alkyl radical], inhibitors of cathepsin K, cathepsin B, and papain, were prepared E.g., 3-[9(S)-benzoylamino-6,10-dioxo-1,2,3,4,7,8,9,10-octahydro-6H-pyridazino[1,2-a][1,2]diazepine-1(S)-carboxamide]-5-methyl-1-benzoyloxyhexane-2-one was prepared

IT 348102-54-5P 348102-56-7P 348102-58-9P 348102-60-3P 348102-62-5P 348102-64-7P 348102-66-9P 348102-68-1P 348102-70-5P 348102-72-7P 348102-74-9P 348102-94-3P

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348102-96-5P 348102-98-7P 348103-00-4P
    348103-02-6P 348103-04-8P 348103-06-0P
    348103-08-2P 348103-10-6P 348103-12-8P
    348103-14-0P 348103-16-2P 348103-18-4P
    348103-20-8P 348103-22-0P 348103-24-2P
    348103-26-4P 348103-28-6P 348103-30-0P
    348103-32-2P 348103-34-4P 348103-36-6P
    348103-38-8P 348103-40-2P 348103-42-4P
    348103-44-6P 348103-46-8P 348103-48-0P
    348103-50-4P 348103-52-6P 348103-54-8P
    348103-56-0P 348103-58-2P 348103-59-3P
     348103-61-7P 348103-63-9P 348103-65-1P
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    348103-76-4P 348103-78-6P 348103-80-0P
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     348104-07-4P 348104-09-6P 348104-11-0P
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     348104-84-7P 348104-86-9P 348104-88-1P
     RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of carboxamide diazepin derivs. and their inhibition of
        cathepsin K, cathepsin B, and papain)
     348102-54-5 CAPLUS
RN
     Hexanoic acid, 6-diazo-4-[[[(1S,9S)-octahydro-9-[(2-methyl-1-
CN
     oxopropy1) amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-
     yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX
NAME)
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RN 348102-56-7 CAPLUS

CN Hexanoic acid, 6-diazo-4-[[[(1s,9s)-octahydro-9-[(3-

methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-

2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

MeO
$$N_2$$
 CH_2

RN 348102-58-9 CAPLUS

CN Hexanoic acid, 6-diazo-4-[[[(1S,9S)-9-[(2-

furanylcarbonyl)amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-

2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348102-60-3 CAPLUS
CN Hexanoic acid, 6-diazo-4-[[[(1S,9S)-octahydro-9-[(4-morpholinylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348102-62-5 CAPLUS

CN Hexanoic acid, 4-[[[(1S,9S)-9-

[[(cyclohexylamino)carbonyl]amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-6-diazo-

5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348102-64-7 CAPLUS

CN Hexanoic acid, 6-diazo-4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348102-66-9 CAPLUS

CN Hexanoic acid, 6-diazo-4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[[2-(2-thienyl)ethyl]amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348102-68-1 CAPLUS

CN Hexanoic acid, 6-diazo-4-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-

2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN 348102-70-5 CAPLUS

CN Hexanoic acid, 6-diazo-4-[[[(15,95)-octahydro-6,10-dioxo-9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-

1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$F_{3}C$$

$$\downarrow \qquad \qquad \downarrow \qquad \downarrow \qquad \qquad \downarrow \qquad$$

RN 348102-72-7 CAPLUS
CN Hexanoic acid, 6-diazo-4-[[[(1S,9S)-octahydro-9-[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348102-74-9 CAPLUS

CN Hexanoic acid, 6-diazo-4-[[((1S,9S)-octahydro-9-[[[5-(3-isoxazolyl)-2-thienyl]sulfonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348102-94-3 CAPLUS
CN Hexanoic acid, 4-[[[(1S,9S)-octahydro-9-[(2-methyl-1-oxopropyl)amino]-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-6[(1phenyl-1H-tetrazol-5-yl)thio]-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348102-96-5 CAPLUS
CN Hexanoic acid, 6-(2-benzothiazolylthio)-4-[[[(1S,9S)-octahydro-9-[(2-methyl-1-oxopropyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin1 yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348102-98-7 CAPLUS

CN Hexanoic acid, 6-[[(4-methoxyphenyl)methyl]thio]-4-[[[(1S,9S)-octahydro-

9-

[(2-methyl-1-oxopropyl)amino]-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-

1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-00-4 CAPLUS

CN Hexanoic acid, 6-(benzoyloxy)-4-[[[(1S,9S)-octahydro-9-[(2-methyl-1-oxopropyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-02-6 CAPLUS

CN 4-Pyridinecarboxylic acid, (3S)-3-[[[(1S,9S)-octahydro-9-[(2-methyl-1-oxopropyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348103-04-8 CAPLUS

CN Hexanoic acid, 6-(acetyloxy)-4-[[[(1S,9S)-octahydro-9-[(2-methyl-1-oxopropyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-06-0 CAPLUS

CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-octahydro-9-[(2-methyl-1-oxopropyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CAINDEX

NAME)

Absolute stereochemistry.

RN 348103-08-2 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[[(1S,9S)-octahydro-9-[(2-methyl-1-oxopropyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-10-6 CAPLUS

CN 1-Piperazinehexanoic acid, 4-[2-(diethylamino)ethyl]- γ -[[[(1S,9S)-octahydro-9-[(2-methyl-1-oxopropyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-12-8 CAPLUS

CN Hexanoic acid, 4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-6-

phenyl-1H-tetrazol-5-yl)thio]-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-14-0 CAPLUS

CN Hexanoic acid, 6-(2-benzothiazolylthio)-4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-16-2 CAPLUS
CN Hexanoic acid, 6-[[(4-methoxyphenyl)methyl]thio]-4-[[[(15,95)-octahydro-9[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin1yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (45)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

RN 348103-18-4 CAPLUS
CN Hexanoic acid, 6-(benzoyloxy)-4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-20-8 CAPLUS

CN 4-Pyridinecarboxylic acid, (3S)-3-[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348103-22-0 CAPLUS

CN Hexanoic acid, 6-(acetyloxy)-4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-24-2 CAPLUS

CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348103-26-4 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-28-6 CAPLUS

CN 1-Piperazinehexanoic acid, 4-[2-(diethylamino)ethyl]- γ -[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-30-0 CAPLUS

CN Hexanoic acid, 6-[(4-methoxyphenyl)thio]-4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-32-2 CAPLUS

CN Hexanoic acid, 4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-6-(2-pyrimidinylthio)-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-34-4 CAPLUS

CN Benzoic acid, 3-(1-cyanoethyl)-, (3S)-3-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348103-36-6 CAPLUS

CN Pentanedioic acid, methyl (3S)-3-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348103-38-8 CAPLUS

CN 1-Piperidinehexanoic acid, γ -[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-(phenylmethyl)-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

RN 348103-40-2 CAPLUS

CN 1-Piperidinehexanoic acid, 3-[(diethylamino)carbonyl]- γ -[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-42-4 CAPLUS

CN Hexanoic acid, 6-(4-fluorophenoxy)-4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-44-6 CAPLUS

CN Hexanoic acid, 4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-6-[(5,6,7,8-tetrahydro-5-oxo-2-naphthalenyl)oxy]-, 2-propenyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-46-8 CAPLUS

CN Hexanoic acid, 6-[2-(acetylamino)phenoxy]-4-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-48-0 CAPLUS

CN Hexanoic acid, 6-[4-[(diethylamino)carbonyl]-2-methoxyphenoxy]-4[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6Hpyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl
ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-50-4 CAPLUS

CN Hexanoic acid, 4-[[(15,95)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-6-

[(1-phenyl-1H-tetrazol-5-yl)thio]-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-52-6 CAPLUS

CN Hexanoic acid, 6-(2-benzothiazolylthio)-4-[[(1S,9S)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)-(9CI)

(CA INDEX NAME)

RN 348103-54-8 CAPLUS

CN Hexanoic acid, 4-[[[(1S,9S)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-6-[[(4-methoxyphenyl)methyl]thio]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-56-0 CAPLUS

CN 4-Pyridinecarboxylic acid, (3S)-3-[[[(1S,9S)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX NAME)

RN 348103-58-2 CAPLUS
CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-59-3 CAPLUS
CN Hexanoic acid, 6-(acetyloxy)-4-[[[(15,95)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (45)-(9CI)

(CA INDEX NAME)

RN 348103-61-7 CAPLUS

CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-63-9 CAPLUS

CN Pentanedioic acid, (3S)-3-[[[(1S,9S)-9-[(2-

furanylcarbonyl)amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-65-1 CAPLUS

CN 1-Piperidinehexanoic acid, γ -[[[(1S,9S)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-(phenylmethyl)-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

RN . 348103-67-3 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[(1S,9S)-9-[(2-furanylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-69-5 CAPLUS

CN Hexanoic acid, 6-[[(4-methoxyphenyl)methyl]thio]-4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-71-9 CAPLUS

CN Hexanoic acid, 6-[(4-methoxyphenyl)thio]-4-[[[(1S,9S)-octahydro-6,10-dioxo-

9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 348103-76-4 CAPLUS

CN Hexanoic acid, 6-(benzoyloxy)-4-[[[(1s,9s)-octahydro-6,10-dioxo-9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

 ${\bf Absolute \ stereochemistry.}$

RN 348103-82-2 CAPLUS

CN Hexanoic acid, 6-(acetyloxy)-4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-84-4 CAPLUS

CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX NAME)

RN 348103-86-6 CAPLUS

CN Pentanedioic acid, methyl (3S)=3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-

1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-88-8 CAPLUS

CN Hexanoic acid, 6-[2-(acetylamino)phenoxy]-4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 348103-90-2 CAPLUS

CN Hexanoic acid, 6-[4-[(diethylamino)carbonyl]-2-methoxyphenoxy]-4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[4-

(trifluoromethyl)phenyl]sulfonyl]am

ino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-,
2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-92-4 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-

1-yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348103-94-6 CAPLUS

CN Hexanoic acid, 4-[[[(1S,9S)-octahydro-9-[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-

6[(1-phenyl-1H-tetrazol-5-yl)thio]-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348103-96-8 CAPLUS
CN Hexanoic acid, 6-[[(4-methoxyphenyl)methyl]thio]-4-[[[(1S,9S)-octahydro-9[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 348103-98-0 CAPLUS
CN Hexanoic acid, 6-(benzoyloxy)-4-[[[(1S,9S)-octahydro-9-[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

348104-01-8 CAPLUS RN CN

4-Pyridinecarboxylic acid, (3S)-3-[[[(1S,9S)-octahydro-9-[(2naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-

a] [1,2] diazepin-1-

yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) INDEX

NAME)

Absolute stereochemistry.

348104-03-0 CAPLUS RN

Hexanoic acid, 6-(acetyloxy)-4-[[[(1S,9S)-octahydro-9-[(2naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2a][1,2]diazepin-1-

yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348104-05-2 CAPLUS

CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-octahydro-9-[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348104-07-4 CAPLUS

CN Pentanedioic acid, methyl (3S)-3-[[[(1S,9S)-octahydro-9-[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA

yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

RN 348104-09-6 CAPLUS

CN Hexanoic acid, 6-[2-(acetylamino)phenoxy]-4-[[[(1S,9S)-octahydro-9-[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-11-0 CAPLUS

CN Hexanoic acid, 6-[4-[(diethylamino)carbonyl]-2-methoxyphenoxy]-4[[[(1S,9S)-octahydro-9-[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6Hpyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl
ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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RN 348104-13-2 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[[(1S,9S)-octahydro-9-[(2-naphthalenylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-15-4 CAPLUS
CN Hexanoic acid, 6-[[(4-methoxyphenyl)methyl]thio]-4-[[[(1S,9S)-octahydro-9[(4-morpholinylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 348104-19-8 CAPLUS
CN Pentanedioic acid, methyl (3S)-3-[[[(1S,9S)-octahydro-9-[(4-morpholinylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin1yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA
INDEX
NAME)

Absolute stereochemistry.

RN 348104-21-2 CAPLUS
CN Hexanoic acid, 4-[[[(1S,9S)-9[[(cyclohexylamino)carbonyl]amino]octahydro6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-6[[(4methoxyphenyl)methyl]thio]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CAINDEX NAME)

RN 348104-23-4 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-

[[(cyclohexylamino)carbonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-25-6 CAPLUS

CN Hexanoic acid, 6-(acetyloxy)-4-[[[(1s,9s)-9-

[[(cyclohexylamino)carbonyl]am

ino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX

yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) NAME)

RN 348104-27-8 CAPLUS
CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-9[[(cyclohexylamino)carbonyl]am
 ino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1 yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA
INDEX
 NAME)

Absolute stereochemistry.

RN 348104-29-0 CAPLUS
CN Pentanedioic acid, (3S)-3-[[[(1S,9S)-9[[(cyclohexylamino)carbonyl]amino]o
ctahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]2,6-dioxo-6-(2-propenyloxy)hexyl methyl ester (9CI) (CA INDEX NAME)

RN 348104-32-5 CAPLUS

CN 1-Piperidinehexanoic acid, γ -[[[(1S,9S)-9-

[[(cyclohexylamino)carbonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-(phenylmethyl)-,

2-propenyl ester, (γS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-34-7 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[[(1S,9S)-9-

[[(cyclohexylamino)carbonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

CN Hexanoic acid, 4-[[(1S,9S)-octahydro-6,10-dioxo-9-[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-6-[(1-phenyl-1H-tetrazol-5-yl)thio]-, 2-propenyl

ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-38-1 CAPLUS

CN Hexanoic acid, 6-(2-benzothiazolylthio)-4-[[(1S,9S)-octahydro-6,10-dioxo-

9-[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 348104-40-5 CAPLUS

CN Hexanoic acid, 6-[[(4-methoxyphenyl)methyl]thio]-4-[[[(15,9S)-octahydro-6,10-dioxo-9-[[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)-(9CI)

(CA INDEX NAME)

RN 348104-42-7 CAPLUS

CN 4-Pyridinecarboxylic acid, (3S)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[(4-

phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA
INDEX

NAME)

Absolute stereochemistry.

RN 348104-45-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX NAME)

RN 348104-47-2 CAPLUS

CN Hexanoic acid, 6-(acetyloxy)-4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-49-4 CAPLUS

CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

RN 348104-51-8 CAPLUS

CN Pentanedioic acid, methyl (3S)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[(4-

phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA
INDEX

NAME)

Absolute stereochemistry.

RN 348104-53-0 CAPLUS

CN 1-Piperidinehexanoic acid, γ -[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-(phenylmethyl)-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-55-2 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[(4-phenoxyphenyl)amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-, 2-propenyl ester, (γS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-57-4 CAPLUS

CN Hexanoic acid, 4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[[2-(2-thienyl)ethyl]amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-6-[(1-phenyl-1H-tetrazol-5-yl)thio]-, 2-propenyl

ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-59-6 CAPLUS

CN Hexanoic acid, 6-(2-benzothiazolylthio)-4-[[(1S,9S)-octahydro-6,10-dioxo-

9-[[[[2-(2-thienyl)ethyl]amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)-(9CI)

(CA INDEX NAME)

RN 348104-61-0 CAPLUS

CN 4-Pyridinecarboxylic acid, (3S)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[[2-

(2-thienyl)ethyl]amino]carbonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1-

yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348104-63-2 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[[2-(2-thienyl)ethyl]amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX NAME)

RN 348104-64-3 CAPLUS

CN Hexanoic acid, 6-(acetyloxy)-4-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[[2-

(2thienyl)ethyl]amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

RN 348104-65-4 CAPLUS

CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[[2-(2-6)-0.5]]]]]]

thienyl)ethyl]amino]carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

NAME)

Absolute stereochemistry.

RN 348104-68-7 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[[(1S,9S)-octahydro-6,10-dioxo-9-[[[[2-(2-thienyl)ethyl]amino]carbonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-,

2-propenyl ester, (γS) - (9CI) (CA INDEX NAME)

RN 348104-70-1 CAPLUS

CN Hexanoic acid, 4-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-6-[(1-phenyl-

1H-tetrazol-5-yl)thio]-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-72-3 CAPLUS

CN Hexanoic acid, 6-(2-benzothiazolylthio)-4-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348104-74-5 CAPLUS

CN Hexanoic acid, 6-[[(4-methoxyphenyl)methyl]thio]-4-[[[(1S,9S)-octahydro-

9-

[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 348104-76-7 CAPLUS

CN 4-Pyridinecarboxylic acid, (3S)-3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

RN 348104-78-9 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348104-80-3 CAPLUS

CN Hexanoic acid, 6-(acetyloxy)-4-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-5-oxo-, 2-propenyl ester, (4S)- (9CI) (CA INDEX NAME)

RN 348104-82-5 CAPLUS

CN 3-Thiopheneacetic acid, (3S)-3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348104-84-7 CAPLUS

CN Pentanedioic acid, methyl (3S)-3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-2,6-dioxo-6-(2-propenyloxy)hexyl ester (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 348104-86-9 CAPLUS

CN 1-Piperidinehexanoic acid, γ -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-(phenylmethyl)-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

RN 348104-88-1 CAPLUS

CN 1-Piperazinehexanoic acid, γ -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- δ -oxo-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-, 2-propenyl ester, (γ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
T.4
     2000:144862 CAPLUS Full-text
AN
DN
     132:180588
     Preparation of (annelated)piperazic acids as caspase inhibitor
TΙ
     intermediates
     Robidoux, Andrea L. C.; Wilson, Jeffrey Douglas; Dieterich, Petra;
IN
Storer,
     Neil; Leonardi, Stefania
     Vertex Pharmaceuticals Incorporated, USA
PA
SO
     PCT Int. Appl., 45 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 3
                      KIND
                            DATE
                                            APPLICATION NO.
                                                              DATE
     PATENT NO.
                                            WO 1999-US19080 19990819
     WO 2000010979
                       A1
                             20000302
PΙ
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         W:
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD,
             MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,
             SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG,
             KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
             ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
             CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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                                                              19980819
     US 6201118
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     US 6177565
                       В1
                             20010123
                                            US 1999-235894
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     AU 9956840
                       A1
                             20000314
                                            AU 1999-56840
                                                              19990819
                                          EP 1999-943814
     EP 1104409
                       A1
                             20010606
                                                              19990819
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     US 2001031862
                       A1
                             20011018
                                            US 2001-789049
                                                              20010220
PRAI US 1998-136339
                             19980819
                       Α
     US 1999-235894
                             19990122
                       Α
     WO 1999-US19080
                       W
                             19990819
OS
     CASREACT 132:180588; MARPAT 132:180588
GΙ
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Title compds., e.g., I (R2 = H, alkyl, aryl, etc.; Z = bond or CH2)[II; R = H, R1 = Z1CO2H, Z1 = (un)substituted (oxo)alkylene] were prepared and cyclized to II (RR1 = COZ1). Thus, Br(CH2)3CHBrCO2CMe3 (preparation given) was cyclocondensed with (PhCH2O2CNH)2 to give I (R2 = CMe3, Z = CH2)(II; R = R1 = CO2CH2Ph) which was deprotected and the product N-acylated with (S)-3-phthalimido-2,6-dioxopyran to give II [R = H, R1 = (S)-HO2CCHR3CH2CH2CO, R3 = phthalimido]. The latter was treated with

SOC12/2,6-lutidine to give, after hydrazinolysis, II [RR1 = (S)-COCHNH2CH2CH2CO].

IT 192756-07-3P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of (annelated)piperazic acids as caspase inhibitor intermediates)

RN 192756-07-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1-

isoquinolinylcarbonyl)amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:386128 CAPLUS Full-text

DN 131:144580

TI An efficient stereoselective synthesis of [3S(1S,9S)]-3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxobutanoic acid, an interleukin converting enzyme (ICE) inhibitor

AU Chen, M. H.; Goel, O. P.; Hyun, J.-W.; Magano, J.; Rubin, J. R.

CS Parke-Davis Pharmaceutical Research Division, Warner-Lambert Company, Ann Arbor, MI, 48105, USA

SO Bioorganic & Medicinal Chemistry Letters (1999), 9(11), 1587-1592 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

GI

AB The title compound (I) is a potent interleukin-1 β -converting enzyme inhibitor. Recently, an efficient chiral synthesis of I was accomplished in our labs. The overall yield of this 18-step stereoselective synthesis was 9.8%.

IT 192755-43-4P 234752-71-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent) (stereoselective preparation of interleukin converting enzyme inhibitor)

RN 192755-43-4 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 234752-71-7 CAPLUS

CN Butanoic acid, 3-[[[(1S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-(methoxymethylamino)-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

IT 174799-23-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (stereoselective preparation of interleukin converting enzyme inhibitor)

RN 174799-23-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
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IN Batchelor, Mark James; Bebbington, David; Bemis, Guy W.; Fridman, Wolf Herman; Gillespie, Roger John; Golec, Julian M. C.; Lauffer, David J.; Livingston, David J.; Matharu, Saroop Singh; Mullican, Michael D.; Murcko,

Mark A.; Murdoch, Robert; Zelle, Robert E.

PA Vertex Pharmaceuticals Incorporated, USA

SO U.S., 189 pp., Cont.-in-part of U.S. Ser. No. 575,641. CODEN: USXXAM

DT Patent

LA English

FAN.	CNT	2							٠,									
		rent .	KIND		DATE			APPLICATION NO.			0.	DATE						
PI	US	s 5874424			Α		19990223			US 1996-598332					19960208			
	US 6008217		217	Α			19991228			US 1995-575641				19951220				
	US	S 6204261 N 182290 D 9722619			B1		20010320			US 1996-761483				19961206				
	IN				A A2 A3		19990306			IN 1996-CA2188				8	19961218			
							1997	0626		WO 1996-US20843					19961220			
	WO	9722619		1997														
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							MD,											
		RW:	ΚE,	LS,	MW,	SD,	SZ,	UG,	ΑT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,
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				NE,	SN,	TD,	ΤG											
		SA 9610798			A		19970707					1996-10798				19961220		
	AU 9715222				A.		19970714 20010628			Al	AU 1997-15222				19961220			
		AU 735075 EP 869967			B2													
	EP				A2		19981014					2 1996-945318			19961220			
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		0.510		SI,			FI,											
		R 9612258 N 1229412 Z 326610			A		19990713 19990922			BR 1996-12258					19961220			
					A					CN 1996-199828				-	19961220			
					A		20000825			NZ 1996-326610					19961220			
	JP 2002507961				T2		20020312			JP 1997-523098					19961220			
		TP 2003137896			A2	_				JP 2002-306094					19961220			
	NO 9802597			A		1998			NO 1998-2597 US 1999-400639					19980605				
		US 6258948 US 6423840			B1		2001								1999			
		J 756253		B1	_	2002						7347		2001				
					B2		2003						6122		2001			
DDAT		2003225269				A1 20031204				U:	5 20	02-5	8522		2002	JT28		
PKAI		1995-575641			_		19951220 19960208											
		1996-598332			A2													
		1996-712878 1996-31495P					1996											
							1996:											
		1996-761483 1997-15222			A		1996: 1996:											
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		JP 1997-523098 JO 1996-US20843			A3 19961220 W 19961220													
		1999-400639			w A3		19961220											
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AN 1999:136764 CAPLUS Full-text

DN 130:196957

TI Preparation of bicyclic peptide derivatives as interleukin-1 β converting enzyme inhibitors

os GI

$$\begin{array}{c}
Y^2 \\
N \\
R^5 \\
R \\
\end{array}$$

$$\begin{array}{c}
N \\
N \\
N \\
N \\
\end{array}$$

$$\begin{array}{c}
O \\
M \\
R \\
R^3
\end{array}$$

$$\begin{array}{c}
R^{15} \\
R^3
\end{array}$$

AB Title compds. I [m = 1-2; R3 = CN, CHO, COCH2-T1-R11, COCH2F, C:NOR9, COAr2; R5 = COR10, CO2R9, CONR102, SO2R9, SO2NHR10, COCH2OR9, COCOR10, R9, H, COCO2R10, COCONR9R10; Y = O, H2; T1 = O, S, S(O), SO2; R9 = Ar3, (un)branched C1-6 alkyl optionally unsatd. and optionally substituted with Ar3; R10 = H, Ar3, C3-6 cycloalkyl, any group R9; R11 = Ar4, (CH2)1-3Ar4, H, COAr4; R15 = OH, OAr3, NHOH, (un)branched C1-6 alkoxy optionally unsatd. and optionally substituted with Ar3, CONH2, OR5, OH, OR9, CO2H; Ar2 = (un)substituted 2-oxazolyl, 2-benzoxazolyl, 2-thiazolyl, 2-benzothiazolyl; Ar3, Ar4 = optionally substituted, nitrogen-containing heteroarom. or heterocyclic group containing 1-3 rings] were prepared as inhibitors of interleukin-1β converting enzyme. Thus, bicyclic peptide derivative II was prepared and shown to have Ki = 13 nM in a UV-visible assay and IC50 = 11000 nM in a peripheral blood mononuclear cell (PBMC) assay.

IT 174799-23-6P 192754-08-8P 192754-09-9P 192755-43-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of bicyclic peptide derivs. as interleukin-1 β converting enzyme inhibitors)

RN 174799-23-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192754-08-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-[[(2,6-dichlorophenyl)methoxy]imino]-, 1,1-dimethylethyl ester, (3S)- (9CI)

(CA

INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 192754-09-9 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-[(2-phenylethoxy)imino]-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 192755-43-4 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

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IT
     174799-04-3P 174799-05-4P 174799-28-1P
     175209-10-6P 175209-11-7P 175209-35-5P
     175209-36-6P 175209-41-3P 175209-48-0P
     175209-61-7P 175209-93-5P 192753-95-0P
     192753-97-2P 192754-02-2P 192754-03-3P
     192754-10-2P 192754-11-3P 192754-50-0P
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     192754-61-3P 192754-76-0P 192754-98-6P
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192756-79-9P 192756-80-2P 192756-81-3P 192756-82-4P 192756-83-5P 192756-84-6P 192756-86-8P 192756-87-9P 192756-88-0P 192756-89-1P 192762-50-8P 220743-36-2P 220743-37-3P 220743-45-3P 220743-47-5P 220743-50-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of bicyclic peptide derivs. as interleukin-1 $\!\beta$ converting enzyme inhibitors)

RN 174799-04-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-05-4 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-

1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

CN Butanoic acid, 3-[[(1s,9s)-9-[(2-fluorobenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 175209-10-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3- / phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-

4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 175209-11-7 CAPLUS

CN Butanoic acid, 3-[[[(15,9S)-octahydro-10-oxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-

4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 175209-35-5 CAPLUS

CN 2-Benzoxazolebutanoic acid, 7-methoxy- β -[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-36-6 CAPLUS

CN 2-Benzoxazolebutanoic acid, 4-methoxy-β-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-41-3 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 175209-48-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-61-7 CAPLUS

CN 2-0xazolebutanoic acid, 5-(2,6-dichlorophenyl)- β -[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

RN 175209-93-5 CAPLUS

CN Pentanoic acid, 5-[[(2-chlorophenyl)methyl]thio]-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-95-0 CAPLUS

CN Pentanoic acid, 3-[[(15,98)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-fluoro-4-oxo-(9CI)

(CA INDEX NAME)

RN 192753-97-2 CAPLUS

CN Propanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-3-cyano-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-02-2 CAPLUS

CN Pentanoic acid, 4-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-03-3 CAPLUS

CN Pentanoic acid, 4-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, (4R)- (9CI)

Absolute stereochemistry. Rotation (-).

RN 192754-10-2 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-[(2,6-dichlorophenyl)methoxy]imino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 192754-11-3 CAPLUS

CN Butanoic acid, 3-[[(15,95)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-[(2-phenylethoxy)imino]-, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 192754-50-0 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-51-1 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-52-2 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-

(benzoylamino) octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 192754-53-3 CAPLUS

CN 2-Oxazolebutanoic acid, 5-(2,6-dichlorophenyl)- β -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-γ-οxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-56-6 CAPLUS

CN 2-Benzoxazolebutanoic acid, 5,7-dichloro- β -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

RN 192754-57-7 CAPLUS

CN 2-Benzoxazolebutanoic acid, β -[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5,7-dichloro- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-59-9 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[[(2-chlorophenyl)methyl]thio]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192754-61-3 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[(2-chlorophenyl)methoxy]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-76-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-10-oxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-98-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,8S,9S)-9-(benzoylamino)octahydro-8-methyl-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-26-3 CAPLUS

CN Pentanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[(1-phenyl-

1Htetrazol-5-yl)thio]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-28-5 CAPLUS

CN Sulfonium, [(3S)-3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-carboxy-2-oxobutyl][(2-chlorophenyl)methyl]methyl-, tetrafluoroborate(1-) (9CI) (CA

INDEX NAME)

CM 1

CRN 192755-27-4

CMF C30 H34 C1 N4 O7 S

Absolute stereochemistry.

CM 2

CRN 14874-70-5

CMF B F4

RN 192755-29-6 CAPLUS

CN Pentanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(2-pyrimidinylthio)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-30-9 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-31-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-32-1 CAPLUS

CN Benzoic acid, 2,6-dimethyl-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 192755-33-2 CAPLUS

CN 1-Naphthalenecarboxylic acid, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-34-3 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-chloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-99-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(2-methylbenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

RN 192756-00-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(2-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-01-7 CAPLUS

CN Butanoic acid, 3-[[[(15,95)-9-[(2-chlorobenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-02-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(2-naphthalenylcarbonyl)amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-03-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1-naphthalenylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-04-0 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-9-[([1,1'-biphenyl]-4-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-05-1 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-6,10-dioxo-9-[(3-thienylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-06-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(2-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-07-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1-isoquinolinylcarbonyl)amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

RN 192756-08-4 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(cyclopropylcarbonyl)amino]octahydro-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
(3S)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-09-5 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(1,3-benzodioxol-5-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-10-8 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(4-chlorobenzoyl)amino]octahydro-6,10-

dioxo-

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-11-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(3,4,5-trimethoxybenzoyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-12-0 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-[[4-(acetylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S)- (9CI) (CA INDEX NAME)

RN 192756-13-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-14-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(methylamino)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-15-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(ethylsulfonyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-16-4 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-[[(1-ethyl-3-methyl-1H-pyrazol-5-yl)carbonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-17-5 CAPLUS

CN Butanoic acid, 3-[[(1s,9s)-9-[(2,4-dimethyl-5-thiazolyl)carbonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3s)- (9CI) (CA INDEX NAME)

RN 192756-19-7 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(6-hydroxy-2-naphthalenyl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-

1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-20-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(cyclohexylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-21-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(phenylsulfonyl)amino]-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

RN 192756-22-2 CAPLUS

CN Butanoic acid, 3-[[[(15,95)-9-[[(dimethylamino)sulfonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-23-3 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-aminooctahydro-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-24-4 CAPLUS

CN Butanoic acid, 3-[[(15,95)-9-[[2-(acetylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

Absolute stereochemistry.

RN 192756-25-5 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(4-aminobenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-26-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(1H-benzotriazol-5-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN, 192756-28-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(1H-benzimidazol-5-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-

1yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-29-9 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-6,10-dioxo-9-[(4-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-30-2 CAPLUS

CN Butanoic acid, 3-[[((1S,9S)-octahydro-6,10-dioxo-9-[(3-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-31-3 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(4-methoxy-2-quinolinyl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin1yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-32-4 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(6-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-33-5 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(8-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 192756-35-7 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[[[4-(dimethylamino)-1-naphthalenyl]carbonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-36-8 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(thieno[2,3-b]thien-2ylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-4oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-37-9 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(4-phenoxybenzoyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

CN Butanoic acid, 3-[[(1S,9S)-9-[(2,6-dichlorobenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-39-1 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1H-imidazol-2-ylcarbonyl)amino]6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-40-4 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1,2,3-thiadiazol-5-ylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-42-6 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[[4-(acetylmethylamino)benzoyl]amino]octahyd
ro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4oxo, (3S)- (9CI) (CA INDEX NAME)

RN 192756-43-7 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-9-[[(1-hydroxy-2-naphthalenyl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-44-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[3-(acetylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-45-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

RN 192756-46-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(4-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-48-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(3-pyridinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-49-3 CAPLUS

CN Butanoic acid, 3-[[(1s,9s)-9-[(3-chlorobenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-50-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(4-hydroxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-51-7 CAPLUS

CN Benzoic acid, 4-hydroxy-, 4-[[[(4S,7S)-4-[[[(1S)-2-carboxy-1-formylethyl]amino]carbonyl]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-7-yl]amino]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

RN 192756-52-8 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-9-[(3,4-difluorobenzoyl)amino]octahydro-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
(3S)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-53-9 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-chloro-4-fluorobenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-54-0 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[4-(methylsulfonyl)benzoyl]amino]6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)- (9CI) (CA INDEX NAME)

RN 192756-55-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-fluorobenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-56-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(4-fluorobenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

RN 192756-57-3 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-9-[(3,4-dichlorobenzoyl)amino]octahydro-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
(3S)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-58-4 CAPLUS
CN Butanoic acid, 3-[[(1S,9S)-9-[(3-chloro-2-methylbenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-59-5 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-9-[(5-chloro-2-methylbenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3s)-(9CI) (CA INDEX NAME)

RN 192756-61-9 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-9-[[[4-methyl-2-[4-(trifluoromethyl)phenyl]-5-thiazolyl]carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-62-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[3-

(dimethylamino)benzoyl]amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

Absolute stereochemistry.

RN 192756-63-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[4-

(dimethylamino)benzoyl]amino]octahydro 6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo,
 (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-65-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(6-methyl-1,3-benzodioxol-5-yl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-66-4 CAPLUS

CN Butanoic acid, 3-[[[(15,98)-9-[(4-acetylbenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI)

(CA INDEX NAME)

RN 192756-68-6 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(3-hydroxy-2-methylbenzoyl)amino]6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-69-7 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[4-hydroxy-3-(4-morpholinylmethyl)benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-70-0 CAPLUS CN Butanoic acid, 3-[[(1S,9S)-9-[[4(aminosulfonyl)benzoyl]amino]octahydro 6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo,
 (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-71-1 CAPLUS CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[4-(hydroxymethyl)benzoyl]amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-73-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(4-amino-3-chlorobenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

RN 192756-74-4 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-9-[(4-amino-3,5-dichlorobenzoyl)amino]octahydr
o-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo, (3s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 C_1
 C_1
 C_1
 C_1
 C_1
 C_1
 C_2
 C_2
 C_2
 C_1
 C_2
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 C_2
 C_2

RN 192756-75-5 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[4-(benzoylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

RN 192756-76-6 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-9-[[4-[(2-methyl-1-oxopropyl)amino]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-77-7 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[4-[(1-oxopropyl)amino]benzoyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-78-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[4-[(phenylacetyl)amino]benzoyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-79-9 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-9-[[4-[(3-methyl-1-oxobutyl)amino]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-

1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-80-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[4-[(1-oxobutyl)amino]benzoyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} n-Pr & & \\ \hline \\ \end{array}$$

192756-81-3 CAPLUS

RN

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[4-

[[(methylamino)carbonyl]amino]

benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-83-5 CAPLUS
CN Butanoic acid, 3-[[(1S,9S)-9-[[4-(benzoyloxy)benzoyl]amino]octahydro-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
(3S)(9CI) (CA INDEX NAME)

CN Butanoic acid, 3-[[(1S,9S)-9-[(3-fluoro-4-methoxybenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-86-8 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9[(phenylacetyl)amino]6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-87-9 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-chloro-4-methoxybenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)-(9CI) (CA INDEX NAME)

RN 192756-88-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-chloro-4-

hydroxybenzoyl)amino]octahydro-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-89-1 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-6,10-dioxo-9-[[4-(phenylmethoxy)benzoyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(oxophenylacetyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 220743-36-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(3-methyl-5-isoxazolyl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 220743-37-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(1-methyl-1H-indol-3-yl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 220743-39-5 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(benzo[b]thien-3-

ylcarbonyl)amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 220743-43-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-benzofuranylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 220743-44-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(2E)-1-oxo-3-(4-pyridinyl)-2-propenyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 220743-45-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1H-indol-3-ylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 220743-47-5 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-9-[[3,4-bis(acetylamino)benzoyl]amino]octahydr

o-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

, (3s)- (9CI) (CA INDEX NAME)

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-6,10-dioxo-9-[[(2E)-1-oxo-3-phenyl-2-

propenyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-

oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 175211-62-8P 192753-72-3P 192753-74-5P

192753-76-7P 192753-79-0P 192753-85-8P

192753-87-0P 192753-91-6P 192753-92-7P

192753-94-9P 192753-96-1P 192754-00-0P

192754-01-1P 220744-52-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation of bicyclic peptide derivs. as interleukin-1 $\!\beta$ converting enzyme inhibitors)

RN 175211-62-8 CAPLUS

CN Pentanoic acid, 5-[[(2-chlorophenyl)methyl]thio]-3-[[[(15,95)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester,

(3S) - (9CI) (CA INDEX NAME)

RN 192753-72-3 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-(1,1-

dimethylethoxy)-2,5-dioxopentyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-74-5 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-5-(1,1-dimethylethoxy)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-76-7 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-

(benzoylamino) octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-(1,1-

dimethylethoxy)-2,5-dioxopentyl ester (9CI) (CA INDEX NAME)

. RN 192753-79-0 CAPLUS

CN 2-Oxazolebutanoic acid, 5-(2,6-dichlorophenyl)- β -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]- γ -oxo-, 1,1-dimethylethyl ester, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-85-8 CAPLUS

CN 2-Benzoxazolebutanoic acid, 5,7-dichloro- β -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, 1,1-dimethylethyl ester, (β S)- (9CI) (CA INDEX NAME)

RN 192753-87-0 CAPLUS

CN 2-Benzoxazolebutanoic acid, β -[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5,7-dichloro- γ -oxo-, 1,1-dimethylethyl ester, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-91-6 CAPLUS

CN Pentanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[[(2-chlorophenyl)methyl]thio]-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

RN 192753-92-7 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[(2-chlorophenyl)methoxy]-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CAINDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-94-9 CAPLUS

Pentanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-fluoro-4-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192753-96-1 CAPLUS

Propanoic acid, 3-[[(1s,9s)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-3-cyano-, methyl ester, (3s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-00-0 CAPLUS

CN Pentanoic acid, 4-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 1,1-dimethylethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-01-1 CAPLUS

CN Pentanoic acid, 4-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 1,1-dimethylethyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 220744-52-5 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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                             20020725
                                             US 2001-886773
PRAI US 1994-261452
                        A2
                             19940617
                        A2
                             19950317
     US 1995-405581
     US 1995-440898
                        A3
                             19950525
                             19950605
     US 1995-465216
                        A3
                        A1
                             19950612
     IN 1995-CA659
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ANSWER 7 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN

L4

EP 1995-925257 A3 19950616 WO 1995-US7617 W 19950616 US 1999-430822 A3 19991029

OS MARPAT 130:66805

Interleukin-1 β converting enzyme inhibitors R1NHX1[(CH2)mT](CH2)gR3 (X1 = CH, N; g = 0, 1; m = 0-2; T = a cyclic group, OH, CF3, COCO2H, CO2H; R1 = R4ZNR5CR6R7CO or substituted derivs., where R4 represents certain ring systems; R5 = H, a cyclic group, alkyl, arylcarbonyl, arylsulfonyl, etc.; CR6R7 form a saturated carbocyclic or heterocyclic ring; R3 = CN, 1-alkenyl, alkoxyiminomethyl) were prepared Thus, N-(N-acetyltyrosinylvalinylpipecolyl)-3-amino-4-oxobutanoic acid was prepared and showed IC50 = 6-11 μ M for inhibition of interleukin-1 β converting enzyme.

175209-10-6P 175209-11-7P 175209-35-5P 175209-36-6P 175209-41-3P 175209-44-6P 175209-48-0P 175209-61-7P 175209-93-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of peptide inhibitors of interleukin-1β converting enzyme)

RN 175209-10-6 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 175209-11-7 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-10-oxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 175209-35-5 CAPLUS

CN 2-Benzoxazolebutanoic acid, 7-methoxy- β -[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

RN 175209-36-6 CAPLUS

CN 2-Benzoxazolebutanoic acid, 4-methoxy- β -[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-41-3 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-44-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI)(CA INDEX NAME)

RN 175209-48-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-61-7 CAPLUS

CN 2-Oxazolebutanoic acid, 5-(2,6-dichlorophenyl)- β -[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-93-5 CAPLUS

CN Pentanoic acid, 5-[[(2-chlorophenyl)methyl]thio]-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

IT 175211-62-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of peptide inhibitors of interleukin-1 β converting enzyme)

RN 175211-62-8 CAPLUS

CN Pentanoic acid, 5-[[(2-chlorophenyl)methyl]thio]-3-[[[(15,95)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
     1997:541852 CAPLUS Full-text
AN
DN
     127:234612
     Preparation of heterocyclyl aspartaldehyde peptide derivatives as
TI
     interleukin-1\beta converting enzyme inhibitors
     Bemis, Guy W.; Golec, Julian M. C.; Lauffer, David J.; Mullican, Michael
IN.
     D.; Murcko, Mark A.; Livingston, David J.
     Vertex Pharmaceuticals, Inc., USA
PΑ
     U.S., 67 pp., Cont.-in-part of U.S. Ser. No. 261,452.
SO
     CODEN: USXXAM
     Patent
DT
     English
LA
FAN.CNT 3
     PATENT NO.
                      KIND
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                                            APPLICATION NO.
                                                             DATE
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                            19970812
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                            19980516
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                       Α
                                                             19950612
                                            ZA 1995-4988
                                                             19950615
     ZA 9504988
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                            19961217
                       AA
                            19951228
                                            CA 1995-2192089
                                                             19950616
     CA 2192089
                            19951228
                                            WO 1995-US7617
                                                             19950616
     WO 9535308
                       A1
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             AM, AT, AU, BB, BG, BR, BY,
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             MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,
             TM, TT
         RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
             LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
             SN, TD, TG
                             19960115
                                            AU 1995-29446
                                                             19950616
     AU 9529446
                       A1
                             19990819
     AU 709114
                       B2
                             19970723
                                            EP 1995-925257
                                                             19950616
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         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT,
SE
                             19970910
                                            CN 1995-194381
                                                             19950616
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                       T2
                             19980428
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                       Α
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                             20020725
                       A2
                             19940617
PRAI US 1994-261452
     US 1995-405581
                       A2
                             19950317
     US 1995-440898
                       Α3
                             19950525
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L4

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US 1995-465216
                        19950605
                  A3
IN 1995-CA659
                        19950612
                  A1
EP 1995-925257
                  A3
                        19950616
WO 1995-US7617
                  W
                        19950616
US 1999-430822
                        19991029
                  A3
MARPAT 127:234612
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OS GI

$$(CJ_2)_{m-T}$$
 $Q = R_{5N}$ X_{5} X_{5}

The present invention relates to novel classes of compds. I [X1 = CH, N;AΒ q = 0, 1; J = independently H, OH, F; <math>m = 0-2; T = Ar3, OH, CF3, COCO2H, CO2H, COCH2OH, CONHOH, SO2NHR, SO3H, P(O)(OH)NH2, CONHCN, OSO3H, CONHSO2R16, PO3H2, P(O) (OH) OR16, P(O) (OH) R16, OPO3H2, OP(O) (OH) OR16, OP(O)(OH)R16, NHPO3H2, NHP(O)(OH)OR16, NHP(O)(OH)R16, COCH:C(OH)CO2H, 5or 6-membered heterocyclic ring; R16 = C1-6 alkyl; R1 = optionally substituted fragment Q; X2 = 0, CH2, NH, S, S(0), SO2; X5 = CH, N; n =0-1, d = 0-2, such that n + d + d = 2; R3 = CN, CH:CHR9, CH:NOR9, (CH2)1-3T1R9, CJ2R9, COR13, COCONR5R10; each R4 = H, Ar1, R9, T1R9, (CH2)1-3T1R9; each T1 = CH:CH, O, S, S(O), SO2, NR10, NR10CO, CO, O2C, CO2, CONR10, O2CNR10, NR10CONR10, SO2NR10, NR10SO2, NR10SO2NR10; R5 = H, Ar1, COAr1, SO2Ar1, R9, CONR9, CO2R9, SO2R9, CONAr1R10, SO2NAr1R10, CONR9R10, SO2NR9R10; R5 = Ar1, SO2Ar1, COR9, CONAr1R10, SO2NAr1R10, CONR9R10, SO2NR9R10; R9 = optionally substituted, straight or branched C1-6 alkyl; R10 = H, C1-6 straight or branched alkyl; R13 = H, Ar1, Ar2, R9, T1R9, (CH2)1-3T1R9; Ar1 = aryl, cycloalkyl, or heterocyclyl group containing 1-3 rings and 3-15 ring atoms; Ar2 = optionally benzo-fused 5-membered heterocyclyl; Ar3 = optionally substituted Ph or 5-membered heterocyclic ring] which are inhibitors of interleukin- 1β converting enzyme. The ICE inhibitors of this invention are characterized by specific structural and physicochem. features. This invention also relates to pharmaceutical compns. comprising these compds. The compds. and pharmaceutical compns. of this invention are particularly well suited for inhibiting ICE activity and consequently, may be advantageously used as agents against interleukin-1 mediated diseases, including inflammatory diseases, autoimmune diseases and neurodegenerative diseases. This invention also relates to methods for inhibiting ICE activity and methods for treating interleukin-1 mediated diseases using the compds. and compns. of this invention.

cyclocondensation of Et 2-aminopyrrolidine-5- carboxylate with 4-ethoxymethylene-2-phenyl-2-oxazolidin-2-one gave 32% pyrrolopyrimidine II. Saponification of II, followed by coupling with tert-Bu (3S)-amino-4-oxobutanoate semicarbazone, diastereomer separation, and deprotection, gave ICE inhibitors III. III and related compds. inhibited ICE with Ki = 0.011 to 35 μM in a UV-visible assay and IC50 = 0.50 to >35 μM in a cell assay.

IT 175209-10-6P 175209-11-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological $\,$

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of heterocyclyl aspartaldehyde peptide derivs. as interleukin- 1β converting enzyme inhibitors)

RN 175209-10-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-

4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 175209-11-7 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-10-oxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-

4-oxo-, (3S)- (9CI) (CA INDEX NAME)

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L4 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:502830 CAPLUS <u>Full-text</u>
DN 127:122000
TI Inhibitors of interleukin-1β converting enzyme
IN Batchelor, Mark J.; Bebbington, David; Bemis, Guy
Herman; Gillespie, Roger J.; Golec, Julian M. C.;
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IN Batchelor, Mark J.; Bebbington, David; Bemis, Guy W.; Fridman, Wolf Herman; Gillespie, Roger J.; Golec, Julian M. C.; Gu, Yong; Lauffer, David J.; Livingston, David J.; Matharu, Saroop S.; Mullican, Michael D.; Murcko, Mark A.; Murdoch, Robert; Nyce, Philip L.; Robidoux, Andrea L. C.; et al.

PA USA

SO PCT Int. Appl., 946 pp. CODEN: PIXXD2

DT Patent LA English FAN.CNT 2

PAN.	PATENT NO.								APPLICATION NO.					DATE				
ΡĪ	WO				A2				WO 1996-US20843					19961220				
	"						AZ,			BG.	BR.	BY.	CA.	СН.	CN.	CII.	CZ.	DE.
		•••	•	•		-	GB,	-	-				-	-				
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		RW:	•	,	•	•	SZ,	•				DE.	DK.	ES.	FI.	FR.	GB.	GR.
			•	•			NL,				-							
			•	NE,	•	•	•	,		,			•	- •			•	
	US					19991228		US 1995-575641				1	1995	1220				
	US			, A					US 1996-598332				2	19960208				
	US	5985863 6204261		Α		19991116			US 1996-712878				8	19960912				
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							FI,											
	BR	326610					19990713											
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		7562								A	J 20	01-7	6122		2001	0928		
PRAI		5 1995-575641 5 1996-598332				19951220												
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		1996			Α		1996							•				
		1996					1996											
		1996					1996											
	AU	1997	-152	22	Α	3	1996											•
	WO	1996	-US2	0843	W		1996	1220										

OS MARPAT 127:122000

AB Compds. R(CH2)nCH(NHR1)(CR22)mR3 [R = NC, R4CH:CH, R4ON:CH, R4CR22, etc. where R2 is independently selected from H, OH, F and R4 is (un)substituted alkyl; R1 = R5NHCHR6CONR7CHR8CO, where CHR6CONR7 is a 2-oxoazepine ring substituted by benzo, pyrido, thieno, or related rings at the 6,7-position and optionally may have O, NH, S, SO, or SO2 at the 5-position, R5 and R8 are H, cyclic group, etc.; R3 = OH, COCOCO2H, CO2H, or any bioisosteric replacement for CO2H; m = 0, 1, 2; n = 0, 1]

were prepared as inhibitors of interleukin-1 β converting enzyme. Thus, [1S,9S(2RS,3S)]-9- benzoylamino-6,10-dioxo-1,2,3,4,7,8,9,10-octahydro-N-(2-benzyloxy-5- oxotetrahydrofuran-3-yl)-6H-pyridazino[1,2-a][1,2]diazepine-1-carboxamide was prepared and shown to have IC50 values of 900 and 600 nM, resp., in the peripheral blood mononuclear cell (PBMC) and whole human blood assays.

IT 192754-50-0P 192755-43-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(inhibitors of interleukin- 1β converting enzyme)

RN 192754-50-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192755-43-4 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 174799-05-4P 174799-23-6P 175209-10-6P 175209-11-7P 175209-35-5P 175209-36-6P 175209-41-3P 175209-44-6P 175209-48-0P 175209-61-7P 192753-76-7P 192754-51-1P

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192754-52-2P 192754-53-3P 192754-54-4P
     192754-56-6P 192754-57-7P 192754-59-9P
     192754-61-3P 192754-76-0P 192754-98-6P
     192755-26-3P 192755-28-5P 192755-30-9P
     192755-31-0P 192755-32-1P 192755-33-2P
     192755-40-1P 192755-94-5P 192755-95-6P
     192755-99-0P 192756-00-6P 192756-01-7P
     192756-02-8P 192756-03-9P 192756-04-0P
     192756-07-3P 192756-10-8P 192756-12-0P
     192756-28-8P 192756-32-4P 192756-36-8P
     192756-44-8P 192756-46-0P 192756-50-6P
     192756-63-1P 192756-67-5P 192756-73-3P
     192756-78-8P 192756-79-9P 192756-90-4P
     192756-91-5P 192759-92-5P 192759-98-1P
     192762-50-8P
     RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (inhibitors of interleukin-1\beta converting enzyme)
RN
     174799-05-4 CAPLUS
CN
     Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-6,10-
     dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-
a][1,2]diazepin-
     1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)
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Absolute stereochemistry. Rotation (-).

RN 174799-23-6 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 175209-10-6 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 175209-11-7 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-octahydro-10-oxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]4-oxo-, (3s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 175209-35-5 CAPLUS 2-Benzoxazolebutanoic acid, 7-methoxy- β -[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1- yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-36-6 CAPLUS

CN 2-Benzoxazolebutanoic acid, 4-methoxy- β -[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino] $-\gamma$ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-41-3 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 175209-44-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 175209-48-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 175209-61-7 CAPLUS

CN 2-Oxazolebutanoic acid, 5-(2,6-dichlorophenyl)- β -[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192753-76-7 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-

(benzoylamino) octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-(1,1-

dimethylethoxy)-2,5-dioxopentyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-51-1 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 192754-52-2 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-

(benzoylamino)octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-carboxy-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-53-3 CAPLUS

CN 2-Oxazolebutanoic acid, 5-(2,6-dichlorophenyl)- β -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

RN 192754-54-4 CAPLUS

CN Pentanoic acid, $3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192754-56-6 CAPLUS

CN 2-Benzoxazolebutanoic acid, 5,7-dichloro- β -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

RN 192754-57-7 CAPLUS

CN 2-Benzoxazolebutanoic acid, β -[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5,7-dichloro-y-oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-59-9 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[[(2-chlorophenyl)methyl]thio]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192754-61-3 CAPLUS

CN Pentanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[(2-chlorophenyl)methoxy]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-76-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-10-oxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192754-98-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,8S,9S)-9-(benzoylamino)octahydro-8-methyl-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-26-3 CAPLUS

CN Pentanoic acid, 3-[[[(1s,9s)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[(1-phenyl-

1Htetrazol-5-yl)thio]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-28-5 CAPLUS

CN Sulfonium, [(3S)-3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-carboxy-2-oxobutyl][(2-chlorophenyl)methyl]methyl-, tetrafluoroborate(1-) (9CI) (CA

INDEX NAME)

CM 1

CRN 192755-27-4

CMF C30 H34 Cl N4 O7 S

Absolute stereochemistry.

CM 2

CRN 14874-70-5

CMF B F4

cci ccs

RN 192755-30-9 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-31-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-32-1 CAPLUS

CN Benzoic acid, 2,6-dimethyl-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-33-2 CAPLUS

CN 1-Naphthalenecarboxylic acid, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 192755-40-1 CAPLUS CN Butanoic acid, 3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2- a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, ethyl ester, $[1S-[1\alpha(R^*),9\alpha]]- (9CI) \quad (CA \ INDEX \ NAME)$

Absolute stereochemistry.

RN 192755-94-5 CAPLUS

CN Butanoic acid, 3-[[[9-[[4-(acetylamino)-3-chlorobenzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

 $[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 192755-95-6 CAPLUS

CN Butanoic acid, 3-[[[9-[(3,5-dichlorobenzoyl)amino]octahydro-6,10-dioxo-6H-

RN 192755-99-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(2-methylbenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-00-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(2-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
(3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-01-7 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(2-chlorobenzoyl)amino]octahydro-6,10-

dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-02-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(2-naphthalenylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-03-9 CAPLUS

CN Butanoic acid, 3-[[[(15,95)-octahydro-9-[(1-naphthalenylcarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S)- (9CI) (CA INDEX NAME)

RN 192756-04-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[([1,1'-biphenyl]-4-

ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-

1yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-07-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1-

isoquinolinylcarbonyl)amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-10-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(4-chlorobenzoyl)amino]octahydro-6,10-

dioxo-

 $6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, \eqno(3S)-(9CI)$

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-12-0 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-[[4-(acetylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-28-8 CAPLUS

CN Butanoic acid, 3-[[[(15,95)-9-[(1H-benzimidazol-5-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-32-4 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(6-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-36-8 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(thieno[2,3-b]thien-2ylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-4oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-44-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[3-(acetylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

Absolute stereochemistry.

RN 192756-46-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(4-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-50-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(4-hydroxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

RN 192756-63-1 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[[4-(dimethylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-67-5 CAPLUS

CN Butanoic acid, 3-[[[octahydro-9-[(1H-indol-2-ylcarbonyl)amino]-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-73-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(4-amino-3-chlorobenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S)- (9CI) (CA INDEX NAME)

RN 192756-78-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[4-[(phenylacetyl)amino]benzoyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-79-9 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[4-[(3-methyl-1-oxobutyl)amino]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-90-4 CAPLUS
CN Butanoic acid, 3-[[[9-[[[(4-chlorophenyl)amino]oxoacetyl]amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-[1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-91-5 CAPLUS

CN Butanoic acid, 3-[[[9-[[(2,6-dimethoxyphenyl)oxoacetyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

 $[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-92-5 CAPLUS

CN Pentanoic acid, $3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

RN 192759-98-1 CAPLUS

CN Pentanoic acid, 3-[[[9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192762-50-8 CAPLUS

CN. Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(oxophenylacetyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 174799-04-3 192759-91-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(inhibitors of interleukin- 1β converting enzyme)

RN 174799-04-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-91-4 CAPLUS

CN Pentanoic acid, 3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-bromo-4-oxo-, $[1S-[1\alpha(R^*),9\alpha]]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CN

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IT
     175211-62-8P 192753-72-3P 192753-74-5P
     192753-79-0P 192753-85-8P 192753-91-6P
     192753-92-7P 192753-94-9P 192753-96-1P
     192754-00-0P 192754-01-1P 192754-08-8P
     192754-09-9P 192754-46-4P 192757-33-8P
     192757-35-0P 192757-38-3P 192757-41-8P
     192757-44-1P 192757-46-3P 192757-47-4P
     192757-48-5P 192757-49-6P 192759-71-0P
     192759-72-1P 192759-74-3P 192759-75-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
     (Reactant or reagent)
        (inhibitors of interleukin-1\beta converting enzyme)
     175211-62-8 CAPLUS
RN
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Pentanoic acid, 5-[[(2-chlorophenyl)methyl]thio]-3-[[[(1S,9S)-octahydro-

6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-72-3 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-3-[[[(1S,9S)-9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-(1,1-

dimethylethoxy)-2,5-dioxopentyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-74-5 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-5-(1,1-dimethylethoxy)-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester (9CI) (CA INDEX NAME)

RN 192753-79-0 CAPLUS

CN 2-Oxazolebutanoic acid, 5-(2,6-dichlorophenyl)- β -[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]- γ -oxo-, 1,1-dimethylethyl ester, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-85-8 CAPLUS

CN 2-Benzoxazolebutanoic acid, 5,7-dichloro- β -[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ -oxo-, 1,1-dimethylethyl ester, (β S)- (9CI) (CA INDEX NAME)

RN 192753-91-6 CAPLUS

CN Pentanoic acid, 3-[[(1s,9s)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[[(2-chlorophenyl)methyl]thio]-4-oxo-, 1,1-dimethylethyl ester, (3s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-92-7 CAPLUS

CN Pentanoic acid, 3-[[((1s,9s)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[(2-chlorophenyl)methoxy]-4-oxo-, 1,1-dimethylethyl ester, (3s)- (9CI) (CA INDEX NAME)

RN 192753-94-9 CAPLUS

CN Pentanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-fluoro-4-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192753-96-1 CAPLUS

CN Propanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-3-cyano-, methyl ester, (3S)- (9CI) (CA INDEX NAME)

RN 192754-00-0 CAPLUS

CN Pentanoic acid, 4-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 1,1-dimethylethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-01-1 CAPLUS

CN Pentanoic acid, 4-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, 1,1-dimethylethyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-08-8 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-[[(2,6-dichlorophenyl)methoxy]imino]-, 1,1-dimethylethyl ester, (3s)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 192754-09-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-[(2-phenylethoxy)imino]-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 192754-46-4 CAPLUS

CN Butanoic acid, 3-[[[9-[(3,5-dichloro-4-methoxybenzoyl)amino]octahydro-6,10-

dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

RN 192757-33-8 CAPLUS

CN 1-Naphthalenecarboxylic acid, 5-(1,1-dimethylethoxy)-3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester, [1S-[1\alpha(R*),9\alpha]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-35-0 CAPLUS

CN 4-Isoxazolecarboxylic acid, 5-methyl-3-phenyl-, 5-(1,1-dimethylethoxy)-3-

[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-38-3 CAPLUS

CN Benzoic acid, 2-phenoxy-, 5-(1,1-dimethylethoxy)-3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

RN 192757-41-8 CAPLUS

CN Benzoic acid, 3-phenoxy-, 5-(1,1-dimethylethoxy)-3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester, [IS-[1\alpha(R*),9\alpha]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-44-1 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-methyl-, 5-(1,1-dimethylethoxy)-3- [[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester, [$1S-[1\alpha(R^*),9\alpha]$]- (9CI) (CA INDEX NAME)

RN 192757-46-3 CAPLUS

CN Pentanoic acid, 3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-diazo-4-oxo-, 1,1-dimethylethyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-47-4 CAPLUS

CN Pentanoic acid, 5-diazo-3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, [$1S-[1\alpha(R^*),9\alpha]$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-48-5 CAPLUS

CN Pentanoic acid, 5-diazo-3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

MeO
$$N_2$$
 OBu-t

RN 192757-49-6 CAPLUS

CN Pentanoic acid, 3-[[[9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-5-diazo-4-oxo-, 1,1-dimethylethyl ester, $[1S-[1\alpha(R^*),9\alpha]]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-71-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 5-(1,1-dimethylethoxy)-3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester, [$1S-[1\alpha(R^*),9\alpha]$]- (9CI) (CA INDEX NAME)

RN 192759-72-1 CAPLUS

CN Benzoic acid, 2,6-dimethyl-, 5-(1,1-dimethylethoxy)-3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2,5-dioxopentyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-74-3 CAPLUS

CN Pentanoic acid, 3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[(1-phenyl-

1H-

tetrazol-5-yl)thio]-, 1,1-dimethylethyl ester, [1S- $[1\alpha(R^*),9\alpha]$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-75-4 CAPLUS /

Pentanoic acid, 3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, 1,1-dimethylethyl ester, [1S-[1\alpha(R*),9\alpha]]-(9CI) (CA INDEX NAME)

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175209-93-5P 192753-87-0P 192753-95-0P
IT
    192753-97-2P 192754-02-2P 192754-03-3P
    192754-10-2P 192754-11-3P 192755-29-6P
    192755-34-3P 192756-96-0P 192757-06-5P
    192757-24-7P 192757-36-1P 192757-39-4P
    192757-42-9P 192757-45-2P 192757-50-9P
    192757-51-0P 192759-69-6P 192759-70-9P
    192759-73-2P 192759-80-1P 192759-81-2P
    192759-82-3P 192759-83-4P 192759-84-5P
    192759-85-6P 192759-86-7P 192759-87-8P
    192759-88-9P 192759-89-0P 192759-90-3P
    192759-93-6P 192759-96-9P 192759-97-0P
    192760-00-2P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (inhibitors of interleukin-1\beta converting enzyme)
    175209-93-5 CAPLUS
RN
     Pentanoic acid, 5-[[(2-chlorophenyl)methyl]thio]-3-[[[(1S,9S)-octahydro-
CN
     6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-
    a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX
NAME)
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Absolute stereochemistry. Rotation (-).

RN 192753-87-0 CAPLUS CN 2-Benzoxazolebutanoic acid, β -[[[(1s,9s)-9-(benzoylamino)octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5,7-dichloro- γ -oxo-, 1,1-dimethylethyl ester, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192753-95-0 CAPLUS

CN Pentanoic acid, 3-[[(15,95)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-fluoro-4-oxo-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 192753-97-2 CAPLUS

CN Propanoic acid, 3-[[(15,95)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-3-cyano-, (3S)-(9CI)

(CA INDEX NAME)

RN 192754-02-2 CAPLUS

CN Pentanoic acid, 4-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-03-3 CAPLUS

CN Pentanoic acid, 4-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-oxo-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192754-10-2 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-[(2,6-dichlorophenyl)methoxy]imino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 192754-11-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-[(2-phenylethoxy)imino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 192755-29-6 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(2-pyrimidinylthio)-, (3S)- (9CI) (CA INDEX NAME)

RN 192755-34-3 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-chloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-96-0 CAPLUS

CN Butanoic acid, 4-(methoxyimino)-3-[[[octahydro-9-[(4-methoxybenzoyl)amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 192757-06-5 CAPLUS

CN Butanoic acid, 3-[[[octahydro-9-[(4-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4- [(phenylmethoxy)imino]-, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 192757-24-7 CAPLUS

CN Butanoic acid, 3-[[[octahydro-9-[(4-hydroxy-3,5-dimethylbenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

 $[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-36-1 CAPLUS

CN 4-Isoxazolecarboxylic acid, 5-methyl-3-phenyl-, 4-carboxy-3-[[[octahydro-9-

[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

RN 192757-39-4 CAPLUS

CN Benzoic acid, 2-phenoxy-, 4-carboxy-3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [1S-[1\alpha(R*),9\alpha]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-42-9 CAPLUS

CN Benzoic acid, 3-phenoxy-, 4-carboxy-3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [1S-[1\alpha(R*),9\alpha]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-45-2 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-methyl-, 4-carboxy-3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [$1S-[1\alpha(R^*),9\alpha]$]- (9CI) (CA INDEX NAME)

RN 192757-50-9 CAPLUS

CN Pentanoic acid, $3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-bromo-4-oxo-, 1,1-dimethylethyl ester, <math>[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 192757-51-0 CAPLUS

CN Pentanoic acid, 5-bromo-3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, [$1S-[1\alpha(R^*),9\alpha]$]- (9CI) (CA INDEX NAME)

RN 192759-69-6 CAPLUS

CN Pentanoic acid, 5-bromo-3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, [$1S-[1\alpha(R^*),9\alpha]$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-70-9 CAPLUS

CN Pentanoic acid, 3-[[[9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-5-bromo-4-oxo-, 1,1-dimethylethyl ester, $[1S-[1\alpha(R^*),9\alpha]]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-73-2 CAPLUS

CN Pentanoic acid, $3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(2-thiazolylthio)-, <math>[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

RN 192759-80-1 CAPLUS

CN 1(6H)-Pyrimidinepentanoic acid, β -[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ ,6-dioxo-, 1,1-dimethylethyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-81-2 CAPLUS

CN 1(6H)-Pyrimidinepentanoic acid, β -[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]- γ ,6-dioxo-, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-84-5 CAPLUS

CN Pentanoic acid, 3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[(1-phenyl-

1H-

tetrazol-5-yl)thio]-, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-85-6 CAPLUS

CN Pentanoic acid, 3-[[[octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3 pyridinyloxy)-, 1,1-dimethylethyl ester, [1S-[1α(R*),9α]] (9CI) (CA INDEX NAME)

RN 192759-86-7 CAPLUS

CN Pentanoic acid, 3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(2 pyrimidinylthio)-, 1,1-dimethylethyl ester, [1S-[1α(R*),9α]] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-87-8 CAPLUS

CN Pentanoic acid, $3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(2-pyrimidinylthio)-, <math>[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-88-9 CAPLUS

CN Pentanoic acid, 3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[(1-phenyl-

1H- tetrazol-5-yl)thio]-, 1,1-dimethylethyl ester, [1S- $[1\alpha(R^*),9\alpha]$]- (9CI) (CA INDEX NAME)

RN 192759-89-0 CAPLUS

CN Pentanoic acid, 3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[(1-phenyl-

1H-

tetrazol-5-yl)thio]-, $[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-90-3 CAPLUS

CN Pentanoic acid, 3-[[[octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, 1,1-dimethylethyl ester, $[1S-[1\alpha(R^*),9\alpha]]$ -(9CI) (CA INDEX NAME)

RN 192759-93-6 CAPLUS CN Pentanoic acid, 3-[[9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2- a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[(1-phenyl-1H-tetrazol-5-yl)thio]-, 1,1-dimethylethyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-96-9 CAPLUS CN Pentanoic acid, $3-[[[9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[(1-phenyl-1H-tetrazol-5-yl)thio]-, <math>[1S-[1\alpha(R^*),9\alpha]]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192759-97-0 CAPLUS CN Pentanoic acid, 3-[[[9-(acetylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2- a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, 1,1-dimethylethyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

RN 192760-00-2 CAPLUS

CN Butanoic acid, 3-[[[9-(benzoylamino)octahydro-10-oxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1 α (R*),9 β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ΙT

174799-28-1P 192756-05-1P 192756-06-2P

192756-08-4P 192756-09-5P 192756-11-9P

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192756-13-1P 192756-14-2P 192756-15-3P
192756-16-4P 192756-17-5P 192756-18-6P
192756-19-7P 192756-20-0P 192756-21-1P
192756-22-2P 192756-23-3P 192756-24-4P
192756-25-5P 192756-26-6P 192756-27-7P
192756-29-9P 192756-30-2P 192756-31-3P
192756-33-5P 192756-34-6P 192756-35-7P
192756-37-9P 192756-38-0P 192756-39-1P
192756-40-4P 192756-41-5P 192756-42-6P
192756-43-7P 192756-45-9P 192756-47-1P
192756-48-2P 192756-49-3P 192756-51-7P
192756-52-8P 192756-53-9P 192756-54-0P
192756-55-1P 192756-56-2P 192756-57-3P
192756-58-4P 192756-59-5P 192756-60-8P
192756-61-9P 192756-62-0P 192756-64-2P
192756-65-3P 192756-66-4P 192756-68-6P
192756-69-7P 192756-70-0P 192756-71-1P
192756-72-2P 192756-74-4P 192756-75-5P
192756-76-6P 192756-77-7P 192756-80-2P
192756-81-3P 192756-82-4P 192756-83-5P
192756-84-6P 192756-85-7P 192756-86-8P
192756-87-9P 192756-88-0P 192756-89-1P
192756-92-6P 192766-55-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
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study); PREP (Preparation); USES (Uses)

(inhibitors of interleukin- 1β converting enzyme)

RN 174799-28-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(2-fluorobenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-05-1 CAPLUS

CN Butanoic acid, 3-[[[(15,95)-octahydro-6,10-dioxo-9-[(3-thienylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (35)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-06-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(2-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-08-4 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(cyclopropylcarbonyl)amino]octahydro-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
(3S)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-09-5 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(1,3-benzodioxol-5-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin1yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-11-9 CAPLUS CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(3,4,5trimethoxybenzoyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-13-1 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-9-[(methoxycarbonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-14-2 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-9-[[(methylamino)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

RN 192756-15-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(ethylsulfonyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-16-4 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[(1-ethyl-3-methyl-1H-pyrazol-5-yl)carbonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-17-5 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-[[(2,4-dimethyl-5-thiazolyl)carbonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-18-6 CAPLUS

CN Butanoic acid, 3-[[[octahydro-9-[[(5-methyl-3-

isoxazolyl) carbonyl]amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

$$[1S-[1\alpha(R^*),9\alpha]]-(9CI)$$
 (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-19-7 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(6-hydroxy-2-naphthalenyl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-20-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(cyclohexylcarbonyl)amino]octahydro-6,10-

Absolute stereochemistry.

RN 192756-21-1 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9[(phenylsulfonyl)amino]6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-22-2 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[[(dimethylamino)sulfonyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

RN 192756-23-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-aminooctahydro-6,10-dioxo-6H-pyridazino[1,2-

a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-24-4 CAPLUS

CN Butanoic acid, 3-[[[(15,95)-9-[[2-(acetylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

Absolute stereochemistry.

RN 192756-25-5 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(4-aminobenzoyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-26-6 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(1H-benzotriazol-5-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-29-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(4-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-30-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(3-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-31-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(4-methoxy-2-quinolinyl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-33-5 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(8-quinolinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-35-7 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[[4-(dimethylamino)-1-naphthalenyl]carbonyl]amino]octahydro-6;10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-37-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(4-phenoxybenzoyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-38-0 CAPLUS

CN Butanoic acid, 3-[[(15,95)-9-[(2,6-dichlorobenzoyl)amino]octahydro-6,10-

 $\label{local_discrete_discre$

(9CI) (CA INDEX NAME)

RN 192756-39-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(1H-imidazol-2-ylcarbonyl)amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-40-4 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-6,10-dioxo-9-[(1,2,3-thiadiazol-5-ylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-41-5 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-9-[[4-

Absolute stereochemistry.

RN 192756-42-6 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-9-[[4-(acetylmethylamino)benzoyl]amino]octahyd
ro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo, (3s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-45-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(3-methoxybenzoyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-47-1 CAPLUS

CN Butanoic acid, $3-[[[9-[(benzo[b]thien-2-y]carbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-48-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(3-pyridinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-49-3 CAPLUS

CN Butanoic acid, 3-[[(1s,9s)-9-[(3-chlorobenzoyl)amino]octahydro-6,10-dioxo-

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-51-7 CAPLUS

CN Benzoic acid, 4-hydroxy-, 4-[[[(4s,7s)-4-[[[(1s)-2-carboxy-1-formylethyl]amino]carbonyl]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-7-yl]amino]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

RN 192756-52-8 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(3,4-difluorobenzoyl)amino]octahydro-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
(3S)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-53-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-chloro-4-

fluorobenzoyl)amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-54-0 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[4-(methylsulfonyl)benzoyl]amino]6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)- (9CI) (CA INDEX NAME)

RN 192756-55-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-fluorobenzoyl)amino]octahydro-6,10-dioxo-

 $6 \mbox{$H$-pyridazino} [1,2-a] [1,2] \mbox{$diazepin-1-yl] carbonyl] amino} -4-oxo-, \eqno(3S)-(9CI)$

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-56-2 CAPLUS

CN Butanoic acid, 3-[[(1s,9s)-9-[(4-fluorobenzoy1)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)-(9CI)

(CA INDEX NAME)

RN 192756-57-3 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[(3,4-dichlorobenzoyl)amino]octahydro-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
(3S)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-58-4 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-9-[(3-chloro-2-methylbenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-59-5 CAPLUS
CN Butanoic acid, 3-[[[(1s,9s)-9-[(5-chloro-2-methylbenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3s)-(9CI) (CA INDEX NAME)

RN 192756-60-8 CAPLUS

CN Butanoic acid, 3-[[[9-[(2-benzofuranylcarbonyl)amino]octahydro-6,10-dioxo-

6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, $[1S-[1\alpha(R^*),9\alpha]]-$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-61-9 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-9-[[[4-methyl-2-[4-(trifluoromethyl)phenyl]-5-thiazolyl]carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-62-0 CAPLUS
CN Butanoic acid, 3-[[(1S,9S)-9-[[3-(dimethylamino)benzoyl]amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-64-2 CAPLUS

CN Butanoic acid, 3-[[[octahydro-6,10-dioxo-9-[[1-oxo-3-(4-pyridinyl)-2-propenyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-

oxo-, $[1S-[1\alpha(R^*),9\alpha]]$ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 192756-65-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[(6-methyl-1,3-benzodioxol-5-yl)carbonyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-66-4 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-9-[(4-acetylbenzoyl)amino]octahydro-6,10-dioxo-

 $6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, \ \, (3S)-(9CI)$

(CA INDEX NAME)

Absolute stereochemistry.

RN 192756-68-6 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-9-[(3-hydroxy-2-methylbenzoyl)amino]-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-69-7 CAPLUS

CN Butanoic acid, 3-[[(1S,9S)-octahydro-9-[[4-hydroxy-3-(4-morpholinylmethyl)benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-70-0 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-9-[[4-(aminosulfonyl)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo(3S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-72-2 CAPLUS

CN Butanoic acid, 3-[[[9-[[3,5-bis(acetylamino)benzoyl]amino]octahydro-6,10-

dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-74-4 CAPLUS

CN Butanoic acid, 3-[[[(15,95)-9-[(4-amino-3,5-

dichlorobenzoyl)amino]octahydr

o-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 $C1$
 S
 CO_2H

RN 192756-75-5 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[4-(benzoylamino)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

RN 192756-76-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[4-[(2-methyl-1-oxopropyl)amino]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-77-7 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[4-[(1-oxopropyl)amino]benzoyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-80-2 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[4-[(1-oxobutyl)amino]benzoyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-81-3 CAPLUS

CN Butanoic acid, 3-[[(1s,9s)-octahydro-9-[[4-

[[(methylamino)carbonyl]amino]

benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-82-4 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[[4-

[(methoxycarbonyl)amino]benzoy

l]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-

4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-83-5 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[[4-(benzoyloxy)benzoyl]amino]octahydro-6,10-

 $\label{local_discrete_discre$

(9CI) (CA INDEX NAME)

RN 192756-84-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-fluoro-4-methoxybenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-85-7 CAPLUS

CN Butanoic acid, $3-[[[octahydro-6,10-dioxo-9-[(1-oxo-3-phenyl-2-propenyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 192756-86-8 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(phenylacetyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI)(CA INDEX NAME)

RN 192756-87-9 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-chloro-4-

methoxybenzoyl)amino]octahydro-

6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-

(3S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-88-0 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(3-chloro-4-hydroxybenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,(3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192756-89-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[4-(phenylmethoxy)benzoyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 192756-92-6 CAPLUS

CN Butanoic acid, 3-[[[9-[[4-(acetylamino)-3,5-dichlorobenzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1\alpha(R*),9\alpha]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192766-55-5 CAPLUS

CN Butanoic acid, $3-[[[9-[[4-(acetyloxy)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

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DN 127:44456

TI Pyridazinodiazepines as a High-Affinity, P2-P3 Peptidomimetic Class of Interleukin-1 β -Converting Enzyme Inhibitor

AU Dolle, Roland E.; Prasad, C. V. C.; Prouty, Catherine P.; Salvino, Joseph M.; Awad, Mohamed M. A.; Schmidt, Stanley J.; Hoyer, Denton; Ross, Tina Morgan; Graybill, Todd L.; Speier, Gary J.; Uhl, Joanne; Miller, Robert; Helaszek, Carla T.; Ator, Mark A.

CS Sanofi Winthrop Inc., Collegeville, PA, 19426, USA

SO Journal of Medicinal Chemistry (1997), 40(13), 1941-1946 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

GΙ

The pyridazinodiazepine-based peptidomimetics are potent time-dependent inactivators of interleukin-1 β converting enzyme (kobs/[I]) = 162,000 to 1,220,000 M-1 s-1. The corresponding aspartic acid aldehyde analogs are potent reversible inhibitors of the enzyme with inhibition consts. ranging from 1-50 nM. All of these inhibitors retain the Pl aspartic acid residue and critical hydrogen-bonding functionality, Pl and P3 NH, which are structural elements previously shown to be required for potent enzyme inhibition by peptide-based inhibitors. In addition, inhibitor I exhibits 10-15% oral bioavailability in the dog.

IT 174799-03-2P 174799-04-3P 174799-05-4P 174799-06-5P 174799-07-6P 174799-10-1P 174799-15-6P 174799-16-7P 174799-17-8P 174799-22-5P 174799-23-6P 174799-24-7P 174799-28-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(pyridazinodiazepines as a high-affinity, P2-P3 peptidomimetic class

of

interleukin- 1β -converting enzyme inhibitor)

RN 174799-03-2 CAPLUS

CN Pentanoic acid, 5-[[1-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-3-[[[9-[[4-[(dimethylamino)methyl]benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,
[1S-[1α(R*),9α]]- (9CI) (CA INDEX NAME)

RN 174799-04-3 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-05-4 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-ali1 2ldiazenin-

1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174799-06-5 CAPLUS CN Pentanoic acid, 3-[[[octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amin o]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[[1-phenyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-07-6 CAPLUS

CN Pentanoic acid, $5-[[1-(4-\text{chlorophenyl})-3-(\text{trifluoromethyl})-1\text{H-pyrazol}-5-yl]oxy]-3-[[[octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6\text{H-pyridazino}[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-10-1 CAPLUS

CN Pentanoic acid, 3-[[9-[[4-[(carboxymethyl)thio]benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[[1-(4-

chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-4-oxo-, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-15-6 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[[octahydro-9-[[4-(4-morpholinylmethyl)benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, $[1S-[1\alpha(R^*),9\alpha]]- (9CI) \quad (CA \ INDEX \ NAME)$

Absolute stereochemistry.

PAGE 1-B

RN 174799-16-7 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[[octahydro-9-[[4-[(4-methyl-

1-

piperazinyl)methyl]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 174799-17-8 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[[octahydro-9-[[4-[(2-methyl-

1H-

imidazol-1-yl)methyl]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

CN Benzenebutanoic acid, $4-[[\{4-[[\{1-(\text{carboxymethyl})-3-[[1-(4-\text{chlorophenyl})-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-2- (trifluoromethyl)-1H-pyrazol-5-yl]oxy]-2- oxopropyl]amino]carbonyl]octahydr o-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-7-yl]amino]carbonyl]-, [4S-[4<math>\alpha$ (R*),7 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

CF3

RN 174799-23-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 174799-24-7 CAPLUS

CN Butanoic acid, $3-[[[9-[[4-(carboxymethoxy)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-28-1 CAPLUS

CN Butanoic acid, 3-[[(1s,9s)-9-[(2-fluorobenzoyl)amino]octahydro-6,10-dioxo-

(CA INDEX NAME)

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ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN
      1996:214750 CAPLUS Full-text
DN
      124:290273
TI
      Preparation of peptide analogs as inhibitors of interleukin-1 beta
      converting enzyme (ICE)
      Bemis, Guy W.; Golec, Julian M. C.; Lauffer, David J.; Mullican, Michael
IN
      D.; Murcko, Mark A.; Livingston, David J.
     Vertex Pharmaceuticals Incorp., USA
PΑ
      PCT Int. Appl., 374 pp.
     CODEN: PIXXD2
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     MARPAT 124:290273
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L4

AΒ Novel classes of compds. are prepared, which are characterized by specific structural and physicochem. features comprising (a) a first and a second hydrogen bonding moiety, each of said moieties being capable of forming a hydrogen bond with a different backbone atom of ICE selected from the carbonyl O and the amide NH group of Arg-341 Ser-339, (b) a first and a second moderately hydrophobic moiety, said moieties each being capable of associating with a sep. binding pocket of ICE when the inhibitor is bound thereto, said binding pocket being selected form the P2, P3, P4, and P' binding pockets, and (c) an electroneg. moiety comprising ≥1 electroneg. atoms, said atoms being attached to the same atom or to adjacent atoms in the moiety and said moiety being capable of forming ≥1 hydrogen bonds or salts bridges with residues in the P1 binding pocket of ICE. These compds. and pharmaceutical compns. of this invention are particularly well suited for inhibiting ICE activity and consequently may be advantageously used as agents against interleukin-1 mediated diseases, including inflammatory diseases, autoimmune diseases and neurodegenerative diseases. Thus, etherification of Me N-tertbutoxycarbonyl-cis-4-hydroxyprolinate with phenol using Ph3P and di-Et azodicarboxylate in THF to Me N-tert-butoxycarbonyl-cis-4phenoxyprolinate followed by deprotection with HCl in EtOAc to Me 4phenoxyprolinate hydrochloride and condensation with Ac-Tyr-Val-OH using 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride, HOBT, and diisopropylethylamine in DMF gave Me N-acetyl-L-tyrosinyl-L-valyl-(4phenoxy)prolinate. Saponification of the latter peptide ester with LiOH in aqueous THF to N-acetyl-L-tyrosinyl-L-valyl-(phenoxy)proline followed by condensation with N-allyloxycarbonyl-4-amino-5-benzyloxy-2oxotetrahydrofuran gave N-[N-acetyl-L-tyrosinyl-L-valyl-(4phenoxy)prolinyl]-4-amino-5-benzyloxy-2-oxotetrahydrofuran (1:1 diastereomer mixture), which underwent hydrogenolysis over Pd(OH)2 in MeOH under H atmospheric to give the title compound (I). In a IL-1 β assay with a mixed population of human peripheral blood mononuclear cells or enriched adherent mononuclear cells, I in vitro showed IC50 of 2.6 and 0.25 μM for inhibiting the processing of pre-IL-1 β by ICE. 175209-10-6P 175209-11-7P 175209-35-5P

175209-36-6P 175209-41-3P 175209-44-6P 175209-48-0P 175209-61-7P 175209-93-5P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of peptide analogs as inhibitors of interleukin-1 beta converting enzyme for treating inflammatory, autoimmune and neurodegenerative diseases)

RN 175209-10-6 CAPLUS

CN Butanoic acid, 3-[[[(15,95)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-

4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 175209-11-7 CAPLUS

CN Butanoic acid, 3-[[[(1s,9s)-octahydro-10-oxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]4-oxo-, (3s)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 175209-35-5 CAPLUS

CN 2-Benzoxazolebutanoic acid, 7-methoxy-β-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

RN 175209-36-6 CAPLUS

CN 2-Benzoxazolebutanoic acid, 4-methoxy- β -[[[(18,98)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]- γ -oxo-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-41-3 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

RN 175209-44-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-octahydro-9-[(methylsulfonyl)amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI)(CA INDEX NAME)

Absolute stereochemistry.

RN 175209-48-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175209-61-7 CAPLUS

CN 2-Oxazolebutanoic acid, $5-(2,6-dichlorophenyl)-\beta-[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-<math>\gamma$ -oxo-, (β S)- (9CI) (CA INDEX NAME)

RN 175209-93-5 CAPLUS

CN Pentanoic acid, 5-[[(2-chlorophenyl)methyl]thio]-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 175211-62-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of peptide analogs as inhibitors of interleukin-1 beta converting enzyme for treating inflammatory, autoimmune and neurodegenerative diseases)

RN 175211-62-8 CAPLUS

CN Pentanoic acid, 5-[[(2-chlorophenyl)methyl]thio]-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[(1-oxo-3-phenylpropyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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L4
     ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
ÀΝ
     1996:190878 CAPLUS Full-text
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     124:261732
ΤI
     Preparation of N-(oxodiazabicýcloalkylcarbonyl)aspartates as
     interleukin-1\beta converting enzyme inhibitors
IN
     Dolle, Roland E.; Chaturvedula, Prasad V.; Morgan, Ross Tina; Schmidt,
     Stanley J.
     Sanofi Winthrop, Inc., USA
PΑ
     PCT Int. Appl., 73 pp.
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$$Q = -HN \xrightarrow{\circ} O \xrightarrow{CF3} CF3$$

$$R^{5}HN \xrightarrow{\circ} O \xrightarrow{CO_{2}R6} O \xrightarrow{N-N} CF3$$

OS

GΙ

MARPAT 124:261732

AB ZNHY [Y = CRR1(CH2)nCO2R2; R = C:NNHCONH2, COR3, etc.; R1 = H or deuterium; R2 = OH, alkoxy, NHOH, etc.; R3 = H, pyrazolyloxymethyl, benzoyloxymethyl, etc.; Z = azabicycllylcarbonyl, etc.; n = 1 or 2] were prepared Thus, pyridazinodiazepinecarboxylate I (R5 = PhCH2O2C, R6 = H)

was amidated and the deprotected product amidated to give I [R5 = 4-(Me2N)C6H4CO, R6 = Q]. Selected I had IC50 of $<10\mu M$ against release of interleukin- 1β from human monocytes in vitro. IT174799-03-2P 174799-04-3P 174799-05-4P 174799-06-5P 174799-07-6P 174799-08-7P 174799-09-8P 174799-10-1P 174799-11-2P 174799-12-3P 174799-13-4P 174799-14-5P 174799-15-6P 174799-16-7P 174799-17-8P 174799-18-9P 174799-19-0P 174799-20-3P 174799-21-4P 174799-22-5P 174799-23-6P 174799-24-7P 174799-25-8P 174799-26-9P 174799-27-0P 174799-28-1P 174799-29-2P 174799-30-5P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of N-(oxodiazabicycloalkylcarbonyl)aspartates as interleukin- 1β converting enzyme inhibitors) RN 174799-03-2 CAPLUS Pentanoic acid, 5-[[1-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-CN yl]oxy]-3-[[[9-[[4-[(dimethylamino)methyl]benzoyl]amino]octahydro-6,10dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-,

Absolute stereochemistry.

 $[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

RN 174799-04-3 CAPLUS
CN Butanoic acid, 3-[[[(1S,9S)-octahydro-6,10-dioxo-9[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

RN 174799-05-4 CAPLUS

CN Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-3-[[[(1S,9S)-octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-

1-yl]carbonyl]amino]-2-oxobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174799-06-5 CAPLUS

CN Pentanoic acid, 3-[[[octahydro-6,10-dioxo-9-

[[(phenylmethoxy)carbonyl]amin

o]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[[1-phenyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

RN 174799-07-6 CAPLUS

CN Pentanoic acid, $5-[[1-(4-\text{chlorophenyl})-3-(\text{trifluoromethyl})-1\text{H-pyrazol-5-yl}] \circ xy]-3-[[[octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6\text{H-pyridazino}[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-08-7 CAPLUS

CN Pentanoic acid, 3-[[[octahydro-6,10-dioxo-9-

[[(phenylmethoxy)carbonyl]amin

o]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-[[1-(2-

pyridinyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-, [1S- $[1\alpha(R^*), 9\alpha]$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-09-8 CAPLUS

CN Pentanoic acid, 3-[[[9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[[1-(4-chlorophenyl)-

3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-4-oxo-, [1S-

Absolute stereochemistry.

RN 174799-10-1 CAPLUS
CN Pentanoic acid, 3-[[[9-[[4-[(carboxymethyl)thio]benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[[1-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-4-oxo-,
[1S-[1\alpha(R*),9\alpha]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-11-2 CAPLUS CN Pentanoic acid, $3-[[[9-[[4-[(2-carboxyethyl)thio]benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-5-[[1-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

CF3

RN 174799-12-3 CAPLUS

CN Pentanoic acid, 5-[[1-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-3-[[[octahydro-9-[[(2-methylpropoxy)carbonyl]amino]-6,10-dioxo-6H-

pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1 α (R*),9 α]]- (9CI) (CA INDEX NAME)

RN 174799-13-4 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[[9-[[4-[(dimethylamino)methyl]benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$Me_2N$$

$$O$$

$$N$$

$$S$$

$$CO_2H$$

$$C1$$

$$C1$$

$$C1$$

$$C1$$

$$C1$$

RN 174799-14-5 CAPLUS

3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-2-

oxopropyl]amino]carbonyl]octahy

dro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-7-yl]amino]carbonyl]-, [4S-[$4\alpha(R^*)$,7 α]]- (9CI) (CA INDEX NAME)

RN 174799-15-6 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[[octahydro-9-[[4-(4-morpholinylmethyl)benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, $[1S-[1\alpha(R^*),9\alpha]]- (9CI) \quad (CA \ INDEX \ NAME)$

Absolute stereochemistry.

PAGE 1-B

RN 174799-16-7 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[[octahydro-9-[[4-[(4-methyl-1-

piperazinyl)methyl]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, $[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 174799-17-8 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[[octahydro-9-[[4-[(2-methyl-

1H-

imidazol-1-yl)methyl]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [1S-[$1\alpha(R^*)$,9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-18-9 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 3-[[[9-[(1H-benzimidazol-5-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-

yl]carbonyl]amino]-4-carboxy-2-oxobutyl ester, [1S- $[1\alpha(R^*), 9\alpha]$]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-19-0 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 3-[[[9-[(1H-benzotriazol-5-ylcarbonyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-carboxy-2-oxobutyl ester, [1S-[1α(R*),9α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-20-3 CAPLUS

CN 1H-Benzotriazole-1-carboxylic acid, 5-[[[4-[[[1-(carboxymethyl)-3-[(2,6-dichlorobenzoyl)oxy]-2-oxopropyl]amino]carbonyl]octahydro-6, <math>10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-7-yl]amino]carbonyl]-, 1-ethyl ester, $[4S-[4\alpha(R^*),7\alpha]]-$ (9CI) (CA INDEX NAME)

__OEt

RN 174799-21-4 CAPLUS

CN lH-Benzimidazole-1-carboxylic acid, $5-[[[4-[[[1-(carboxymethyl)-3-[(2,6-dichlorobenzoyl)oxy]-2-oxopropyl]amino]carbonyl]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-7-yl]amino]carbonyl]-, 1-ethyl ester, [4S-[4<math>\alpha$ (R*),7 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

__OEt

RN 174799-22-5 CAPLUS
CN Benzenebutanoic acid, 4-[[[4-[[[1-(carboxymethyl)-3-[[1-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-2-oxopropyl]amino]carbonyl]octahydr

o-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-7-yl]amino]carbonyl]-, [4S-[4 α (R*),7 α]]- (9CI) (CA INDEX NAME)

PAGE 1-B

CF3

RN 174799-23-6 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-24-7 CAPLUS

CN Butanoic acid, $3-[[[9-[[4-(carboxymethoxy)benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

RN 174799-25-8 CAPLUS

CN Benzoic acid, 2,6-dichloro-, 4-carboxy-3-[[[octahydro-10-oxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-2-oxobutyl ester, [1S-[1\alpha(R*),9\alpha]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-26-9 CAPLUS

CN Pentanoic acid, $5-[[1-(5-\text{chloro}-2-\text{pyridinyl})-3-(\text{trifluoromethyl})-1H-\text{pyrazol}-5-yl]\text{oxy}]-3-[[[\text{octahydro}-6,10-\text{dioxo}-9-[[(\text{phenylmethoxy})\text{carbonyl}]\text{amino}]-6H-pyridazino}[1,2-a][1,2]\text{diazepin}-1-yl]\text{carbonyl}]\text{amino}]-4-oxo-, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-27-0 CAPLUS

CN Pentanoic acid, 3-[[[9-[[4[(dimethylamino)methyl]benzoyl]amino]octahydro-6,10-dioxo-6Hpyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5[[1-(2-pyridinyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-,
[1S-[1\(a(R^*),9\(a\text{a})]-(9\text{CI}) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-28-1 CAPLUS

CN Butanoic acid, 3-[[[(1S,9S)-9-[(2-fluorobenzoyl)amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, (3S)- (9CI)(CA INDEX NAME)

Absolute stereochemistry.

RN 174799-29-2 CAPLUS

CN Butanoic acid, $3-[[[octahydro-6,10-dioxo-9-[(2-pyridinylcarbonyl)amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, <math display="block">[1S-[1\alpha(R^*),9\alpha]]-(9CI) \quad (CA \ INDEX \ NAME)$

Absolute stereochemistry.

RN 174799-30-5 CAPLUS

CN Butanoic acid, 3-[[[octahydro-9-[[4-[(4-methyl-1-piperazinyl)methyl]benzoyl]amino]-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, [1S-[1\alpha(R*),9\alpha]]-(9CI) (CA INDEX NAME)

IT 174799-33-8P 174799-34-9P 174799-35-0P 174799-36-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-(oxodiazabicycloalkylcarbonyl)aspartates as interleukin-1 β converting enzyme inhibitors)

RN 174799-33-8 CAPLUS

CN Pentanoic acid, $5-[[1-(4-\text{chlorophenyl})-3-(\text{trifluoromethyl})-1\text{H-pyrazol}-5-yl]\text{oxy}]-3-[[[\text{octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino}]-6\text{H-pyridazino}[1,2-a][1,2]diazepin-1-yl]carbonyl]amino}]-4-oxo-, 1,1-dimethylethyl ester, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-34-9 CAPLUS

CN Pentanoic acid, $3-[[(9-aminooctahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl)carbonyl]amino]-5-[[1-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-5-yl]oxy]-4-oxo-, 1,1-dimethylethyl ester, monohydrochloride, <math>[1S-[1\alpha(R^*),9\alpha]]-(9CI)$ (CA INDEX NAME)

RN 174799-35-0 CAPLUS

CN Pentanoic acid, $5-[[1-(4-\text{chlorophenyl})-3-(\text{trifluoromethyl})-1\text{H-pyrazol}-5-yl]\text{oxy}]-3-[[[9-[[4-[(dimethylamino)methyl]benzoyl]amino]octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, [1S-[1<math>\alpha$ (R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174799-36-1 CAPLUS

CN Hexanoic acid, 6-[(aminocarbonyl)hydrazono]-3-[[[octahydro-6,10-dioxo-9-[[(phenylmethoxy)carbonyl]amino]-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-, 1,1-dimethylethyl ester, [1S-[1 α (3R*),9 α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

Beilstein Records (BRN):

8372336

Autonom Name (AUN):

3-<(9-benzoylamino-6,10-dioxo-octahydro-pyridazino<1,2-a><1,2>diazepine-1-carbonyl)-amino>-N-methoxy-N-methyl-

succinamic acid tert-butyl ester

C27 H37 N5 O8

Molec. Formula (MF):
Molecular Weight (MW):

Molecular Weight (MW):
Lawson Number (LN):

File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):

Tautomer ID (TAUTID):

Entry Date (DED):
Update Date (DUPD):

559.62

29859, 10581, 3625, 3487, 318, 289

Stereo compound heterocyclic

7107718 7902041 2000/03/08

2000/03/08

Reference(s):

 Chen, M. H.; Goel, O. P.; Hyun, J.-W.; Magano, J.; Rubin, J. R., Bioorg.Med.Chem.Lett., CODEN: BMCLE8, 9(11), <1999>, 1587 - 1592; BABS-6189425 Beilstein Records (BRN):

8368830

Autonom Name (AUN):

3-<(9-benzoylamino-6,10-dioxo-octahydro-

pyridazino<1,2-a><1,2>diazepine-1carbonyl)-amino>-4-oxo-butyric acid

tert-butyl ester

Molec. Formula (MF):

C25 H32 N4 O7

Molecular Weight (MW):

500.55

Lawson Number (LN):

29859, 10581, 3614, 318

File Segment (FS):
Compound Type (CTYPE):

Stereo compound heterocyclic

Constitution ID (CONSID):

7104430 7901073

Tautomer ID (TAUTID): Entry Date (DED):

2000/03/08

Update Date (DUPD): 2000/03/08

Reference(s):

 Chen, M. H.; Goel, O. P.; Hyun, J.-W.; Magano, J.; Rubin, J. R., Bioorg.Med.Chem.Lett., CODEN: BMCLE8, 9(11), <1999>, 1587 - 1592; BABS-6189425

L7 ANSWER 3 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):
Molec. Formula (MF):

Molecular Weight (MW):

Lawson Number (LN): File Segment (FS):

Compound Type (CTYPE):

Constitution ID (CONSID):
Tautomer ID (TAUTID):

Beilstein Citation (BSO):

Entry Date (DED):
Update Date (DUPD):

7791359

C34 H32 C1 F3 N6 O10 S

809.17

29859, 28329, 16436, 11689, 3616, 1774

Stereo compound

heterocyclic

6647679 7373455

6-25

1998/03/03 1998/03/03

L7 ANSWER 4 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7791282 C36 H36 Cl F3 N6 O10 Molec. Formula (MF): Molecular Weight (MW): 805.16 Lawson Number (LN): 29859, 28329, 16436, 11187, 3616 File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 6648049 Tautomer ID (TAUTID): 7373231 Beilstein Citation (BSO): 6-25

Entry Date (DED): 1998/03/03 Update Date (DUPD): 1998/03/03

L7 ANSWER 5 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):
Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):

Entry Date (DED):
Update Date (DUPD):

· 7791183

C35 H37 C1 F3 N7 O8

776.17

29859, 28329, 16436, 16047, 3616, 2817

Stereo compound heterocyclic

6646975 7372503 6-25

1998/03/03 1998/03/03

ANSWER 6 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN L7

Beilstein Records (BRN): Molec. Formula (MF):

7791095 C36 H42 Cl2 N6 O9

Molecular Weight (MW):

773.67

Lawson Number (LN): File Segment (FS):

Compound Type (CTYPE):

Constitution ID (CONSID):

7373666 Tautomer ID (TAUTID):

Beilstein Citation (BSO):

Entry Date (DED):

Update Date (DUPD):

29859, 28000, 16047, 10584, 3616, 2817

Stereo compound

heterocyclic

6647412

6-25

1998/03/03

1998/03/03

L7 ANSWER 7 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7791046
Molec. Formula (MF): C33 H32 Cl F3 N6 O9

Molecular Weight (MW): 749.10

Lawson Number (LN): 29859, 28329, 16436, 5228, 3616, 1762

File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic

Constitution ID (CONSID): 6646554
Tautomer ID (TAUTID): 7370899
Beilstein Citation (BSO): 6-25
Entry Date (DED): 1998/03

Entry Date (DED): 1998/03/03 Update Date (DUPD): 1998/03/03

L7 ANSWER 8 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7790974 C35 H39 C12 N5 O10 Molec. Formula (MF): 760.63 Molecular Weight (MW): 30824, 29859, 16047, 10584, 3616 Lawson Number (LN): File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 6647328 Tautomer ID (TAUTID): 7373590 6-27 Beilstein Citation (BSO): 1998/03/03 Entry Date (DED): Update Date (DUPD): 1998/03/03

L7 ANSWER 9 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7790944 C35 H36 C12 N6 O9 Molec. Formula (MF): Molecular Weight (MW): 755.61 29859, 28030, 16047, 10584, 3616 Lawson Number (LN): File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 6646784 7374141 Tautomer ID (TAUTID): Beilstein Citation (BSO): 6-25 1998/03/03 Entry Date (DED): Update Date (DUPD): 1998/03/03

L7 ANSWER 10 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):

Molec. Formula (MF): C33 H33 F3 N6 O9.

Molecular Weight (MW): 714.65

Lawson Number (LN): 29859, 28329, 16435, 5228, 3616, 1762

7790905

File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic

Constitution ID (CONSID): 6645676 Tautomer ID (TAUTID): 7370682 Beilstein Citation (BSO): 6-25

Beilstein Citation (BSO): 6-25 Entry Date (DED): 1998/03/03 Update Date (DUPD): 1998/03/03

L7 ANSWER 11 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

7790071 Beilstein Records (BRN): Molec. Formula (MF): C31 H32 C12 N4 O10 Molecular Weight (MW): 691.52 Lawson Number (LN): 29859, 10584, 5228, 3616, 1762 File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 6644745 Tautomer ID (TAUTID): 7371873 Beilstein Citation (BSO): 6-25 Entry Date (DED): 1998/03/03 Update Date (DUPD): 1998/03/03

L7 ANSWER 12 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7787164 C23 H26 N4 O10 Molec. Formula (MF): 518.48 29859, 11694, 3614, 1771 Molecular Weight (MW): Lawson Number (LN): File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 6637771 Tautomer ID (TAUTID): 7371033 Beilstein Citation (BSO): 6-25 Entry Date (DED): 1998/03/03 Update Date (DUPD): 1998/03/03

L7 ANSWER 13 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7785794 C22 H26 N4 O8 Molec. Formula (MF): Molecular Weight (MW): 474.47 29859, 5228, 3614, 1762 Lawson Number (LN): File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 6632614 Tautomer ID (TAUTID): 7365353 Beilstein Citation (BSO): 6-25 Entry Date (DED): 1998/03/03 Update Date (DUPD): 1998/03/03

L7 ANSWER 14 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7785257 Molec. Formula (MF): C21 H23 F N4 O7 Molecular Weight (MW): 462.43 29859, 10582, 3614 Lawson Number (LN): File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 6633495 Tautomer ID (TAUTID): 7367962 Beilstein Citation (BSO): 6-25 Entry Date (DED): 1998/03/03 Update Date (DUPD): 1998/03/03

L7 ANSWER 15 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

7784055 Beilstein Records (BRN): Chemical Name (CN): PD 194035 Molec. Formula (MF): C21 H24 N4 O7 Molecular Weight (MW): 444.44 Lawson Number (LN): 29859, 10581, 3614 File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 6629728 Tautomer ID (TAUTID): 7367706 Beilstein Citation (BSO): 6-25 Entry Date (DED): 1998/03/03 Update Date (DUPD): 2000/03/07

Reference(s):

 Chen, M. H.; Goel, O. P.; Hyun, J.-W.; Magano, J.; Rubin, J. R., Bioorg.Med.Chem.Lett., CODEN: BMCLE8, 9(11), <1999>, 1587 - 1592; BABS-6189425

Reference(s):

1. Chen, M. H.; Goel, O. P.; Hyun, J.-W.; Magano, J.; Rubin, J. R., Bioorg.Med.Chem.Lett., CODEN: BMCLE8, 9(11), <1999>, 1587 - 1592; BABS-6189425

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ANSWER 1 OF 1 MARPAT COPYRIGHT 2004 ACS on STN
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     126:8707 MARPAT Full-text
AN
     Preparation of beta-sheet mimetics of peptides or proteins as inhibitors
TI
     of biologically active peptides or proteins
     Kahn, Michael
IN
     Molecumetics Ltd., USA
PΑ
SO
     PCT Int. Appl., 158 pp.
     CODEN: PIXXD2
     Patent
DT
     English
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     WO 9630035
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     US 1998-9665
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GΙ
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There are disclosed β -sheet mimetics [I; R1 - R3 = amino acid side chain AB moiety or its derivative; A = CO, (CH2)1-4, (CH2)1-2-O, (CH2)1-2-S; B =N, CH; C = CO, (CH2)1-3, O, S, O(CH2)1-2, S(CH2)1-2; Y, Z = the remainder of the mol.; or any 2 adjacent CH groups of the bicyclic ring may form a double bond] and methods relating to the same for imparting or stabilizing the β -sheet structure of a peptide, protein or mol. one aspect, the β -sheet mimetics are covalently attached at the end or within the length of the peptide or protein. The β -sheet mimetics have utility as inhibitors of one or more of proteases, kinases, CAAX motif (Ras prenylation of the Cys within its C-terminal CAAX sequence by farnesyl transferase, wherein "A" is defined as an amino acid with a hydrophobic side chain and "X" is another amino acid), peptides binding to SH2 domains, and MHC-I and/or MHC-II (major histocompatibility complex class I and class II) presentation of peptides to T cell receptors in warm-blooded animals. Thus, azabicyclo[4.3.0]nonane derivative (II; R = Boc, R4 = OH) (preparation given) was condensed with benzothiazolylarginol derivative (H-Q.CF3CO2H; R5 = Q1, Z = CHOH) using 1-ethyl-3-(3- dimethylaminopropyl) carbodiimide hydrochloride, HOBt, and (Me2CH) 2NEt in THF to give arginol derivative II (R = Boc, R4 = Q, R5 = Q1 Z = CHOH), which was oxidized by Dess-Martin periodinane in CH2Cl2 to arginine derivative II (R = Boc, R4 = Q, R5 = Q1 Z = C0) and deprotected 95% aqueous CF3CO2H and thioanisole at room temperature for 20 h to give, after HPLC purification, the β -sheet mimetic II (R = H, R4 = Q, R5 = H, Z = CO). The latter compound in vitro inhibited various serine proteases such as thrombin, factor VII, factor X, factor XI, urokinase, thrombin-thrombomodulin complex, activated protein C, plasmin, tissue plasminogen activator, trypsin, and tryptase, e.g. with Ki of 8.50 + 10-11 M for thrombin.

MSTR 1

$$G5 - NH - G15 - G7$$
 $G2 = N$
 $G7 = 80$
 $G8 = (1-4) CH2$
 $G12 = (1-3) 24$
 $G2 = G13$

 $G15 = 7-15 \ 2-11$

$$G29 = 162$$

G31 = 157

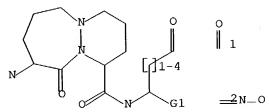
MPL: claim 1

NTE: substitution is restricted

NTE: additional double bond formation possible

STE: 443 - D

=> d l1; d his; log y L1 HAS NO ANSWERS L1 STR



G1 CN, [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

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FILE 'REGISTRY' ENTERED AT 15:59:43 ON 04 MAR 2004

L1 STRUCTURE UPLOADED

L2 16 S L1

L3 344 S L1 FUL

FILE 'CAPLUS' ENTERED AT 16:00:46 ON 04 MAR 2004

L4 12 S L3

FILE 'BEILSTEIN' ENTERED AT 16:02:07 ON 04 MAR 2004

L5 1 S L1

L6 15 S L1 FUL

L7 15 S L6 NOT L4

FILE 'MARPAT' ENTERED AT 16:03:14 ON 04 MAR 2004

Ĺ8 1 S L1

L9 10 S L1 FUL

L10 1 S L9 NOT L4

COST IN U.S. DOLLARS	SINCE FILE	\mathtt{TOTAL}
	ENTRY	SESSION
FULL ESTIMATED COST	114.71	519.91
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.66	-8.98

STN INTERNATIONAL LOGOFF AT 16:05:04 ON 04 MAR 2004

elected compound

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1999:136764 CAPLUS Full-text
AN
     130:196957
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тT
     Preparation of bicyclic peptide derivatives as interleukin-1\beta
     converting enzyme inhibitors
     Batchelor, Mark James; Bebbington, David; Bemis, Guy W.; Fridman, Wolf
IN
     Herman; Gillespie, Roger John; Golec, Julian M. C.; Lauffer, David J.;
     Livingston, David J.; Matharu, Saroop Singh; Mullican, Michael D.;
     Murcko, Mark A.; Murdoch, Robert; Zelle, Robert E.
     Vertex Pharmaceuticals Incorporated, USA
PA
SO
     U.S., 189 pp., Cont.-in-part of U.S. Ser. No. 575,641.
     CODEN: USXXAM
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LΑ
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ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

L4

$$\begin{array}{c} Y^2 \\ N \\ R^5 N \\ O \\ N \\ R^3 \end{array}$$

Title compds. I [m = 1-2; R3 = CN, CHO, COCH2-T1-R11, COCH2F, C:NOR9, COAr2; R5 = COR10, CO2R9, CONR102, SO2R9, SO2NHR10, COCH2OR9, COCOR10, R9, H, COCO2R10, COCONR9R10; Y = O, H2; T1 = O, S, S(O), SO2; R9 = Ar3, (un)branched C1-6 alkyl optionally unsatd. and optionally substituted with Ar3; R10 = H, Ar3, C3-6 cycloalkyl, any group R9; R11 = Ar4, (CH2)1-3Ar4, H, COAr4; R15 = OH, OAr3, NHOH, (un)branched C1-6 alkoxy optionally unsatd. and optionally substituted with Ar3, CONH2, OR5, OH, OR9, CO2H; Ar2 = (un)substituted 2-oxazolyl, 2-benzoxazolyl, 2-thiazolyl, 2-benzothiazolyl; Ar3, Ar4 = optionally substituted, nitrogen-containing heteroarom. or heterocyclic group containing 1-3 rings] were prepared as inhibitors of interleukin-1β converting enzyme. Thus, bicyclic peptide derivative II was prepared and shown to have Ki = 13 nM in a UV-visible assay and IC50 = 11000 nM in a peripheral blood mononuclear cell (PBMC) assay.

IT 192755-30-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of bicyclic peptide derivs. as interleukin-1 β converting enzyme inhibitors)

RN 192755-30-9 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, (3S)- (9CI) (CA INDEX NAME)

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ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN
     1997:502830 CAPLUS Full-text
DN
     127:122000
TI
     Inhibitors of interleukin-1\beta converting enzyme
     Batchelor, Mark J.; Bebbington, David; Bemis, Guy W.; Fridman, Wolf
IN
     Herman; Gillespie, Roger J.; Golec, Julian M. C.; Gu, Yong; Lauffer,
     David J.; Livingston, David J.; Matharu, Saroop S.; Mullican, Michael
     D.; Murcko, Mark A.; Murdoch, Robert; Nyce, Philip L.; Robidoux, Andrea
     L. C.; et al.
PA
     USA
SO
     PCT Int. Appl., 946 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 2
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO. DATE
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                            19961220
OS
     MARPAT 127:122000
     Compds. R(CH2) nCH(NHR1) (CR22) mR3 [R = NC, R4CH:CH, R4ON:CH, R4CR22, etc.
AB
     where R2 is independently selected from H, OH, F and R4 is
     (un) substituted alkyl; R1 = R5NHCHR6CONR7CHR8CO, where CHR6CONR7 is a 2-
     oxoazepine ring substituted by benzo, pyrido, thieno, or related rings
     at the 6,7-position and optionally may have O, NH, S, SO, or SO2 at the
     5-position, R5 and R8 are H, cyclic group, etc.; R3 = OH, COCOCO2H,
     CO2H, or any bioisosteric replacement for CO2H; m = 0, 1, 2; n = 0, 1
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L4

were prepared as inhibitors of interleukin-1 β converting enzyme. Thus, [1S,9S(2RS,3S)]-9- benzoylamino-6,10-dioxo-1,2,3,4,7,8,9,10-octahydro-N-(2-benzyloxy-5- oxotetrahydrofuran-3-yl)-6H-pyridazino[1,2-a][1,2]diazepine-1-carboxamide was prepared and shown to have IC50 values of 900 and 600 nM, resp., in the peripheral blood mononuclear cell (PBMC) and whole human blood assays.

IT 192755-30-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (inhibitors of interleukin-1 β converting enzyme)

RN 192755-30-9 CAPLUS

CN Pentanoic acid, 3-[[[(1S,9S)-9-(benzoylamino)octahydro-6,10-dioxo-6H-pyridazino[1,2-a][1,2]diazepin-1-yl]carbonyl]amino]-4-oxo-5-(3-pyridinyloxy)-, (3S)- (9CI) (CA INDEX NAME)

=> d 11; d his; log y
L1 HAS NO ANSWERS
L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

(FILE 'HOME' ENTERED AT 10:10:56 ON 04 MAR 2004)

FILE 'REGISTRY' ENTERED AT 10:11:05 ON 04 MAR 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 1 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:11:55 ON 04 MAR 2004

L4 2 S L3

FILE 'BEILSTEIN' ENTERED AT 10:12:27 ON 04 MAR 2004

L5 0 S L1 FUL

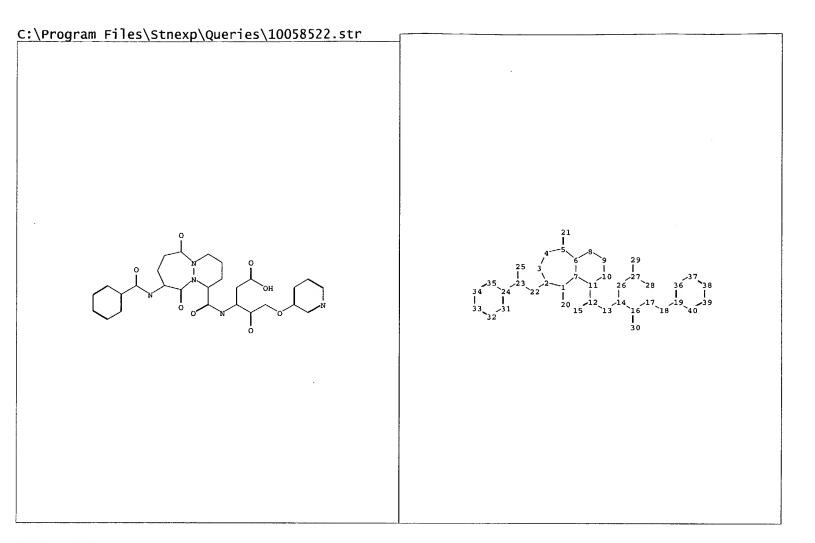
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L6 0 S L1

L7 0 S L1 FUL

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
FULL ESTIMATED COST	ENTRY 109.42	SESSION 275.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY 0.00	SESSION -1.39

STN INTERNATIONAL LOGOFF AT 10:13:14 ON 04 MAR 2004



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ring nodes :
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ring bonds :
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Match level:
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom